



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:32 AM UTC

PDB ID : 2WW3 / pdb_00002ww3
Title : Structure of the Family GH92 Inverting Mannosidase BT3990 from Bacteroides
thetaiotaomicron VPI-5482 in complex with thiomannobioside
Authors : Suits, M.D.L.; Zhu, Y.; Thompson, A.J.; Gilbert, H.J.; Davies, G.J.
Deposited on : 2009-10-21
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

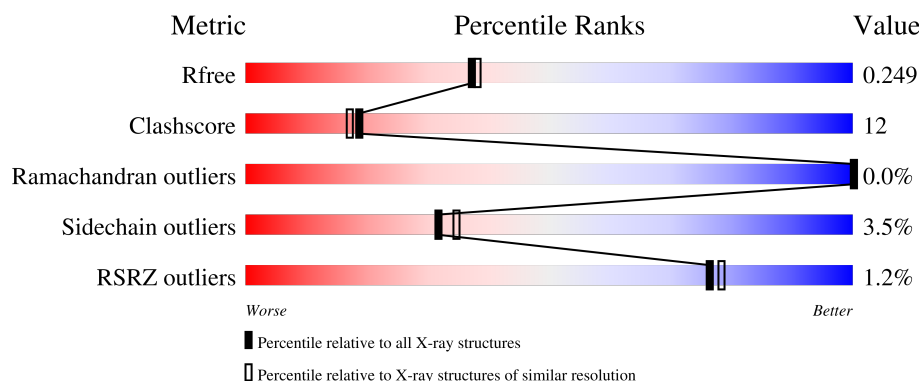
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



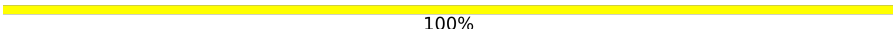
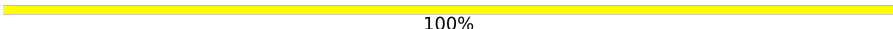
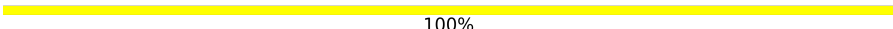
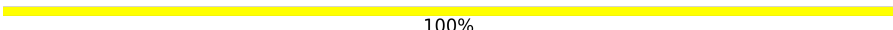
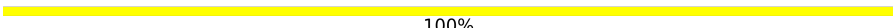
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	744	 81% 17% ..
1	B	744	 5% 70% 26% ..
1	C	744	 83% 15% ..
1	D	744	 % 77% 20% ..
1	E	744	 82% 14% ..

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Mol	Chain	Length	Quality of chain
1	F	744	 78%19%..
2	G	2	 100%
2	H	2	 100%
2	I	2	 100%
2	J	2	 100%
2	K	2	 50%50%
2	L	2	 100%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 37131 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 PUTATIVE ALPHA-1,2-MANNOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	736	Total	C	N	O	S	0	0	0
			5957	3818	981	1125	33			
1	B	736	Total	C	N	O	S	0	0	0
			5937	3806	979	1119	33			
1	C	736	Total	C	N	O	S	0	0	0
			5949	3814	980	1122	33			
1	D	738	Total	C	N	O	S	0	0	0
			5946	3809	977	1127	33			
1	E	736	Total	C	N	O	S	0	1	0
			5945	3811	975	1126	33			
1	F	738	Total	C	N	O	S	0	0	0
			5948	3814	978	1123	33			

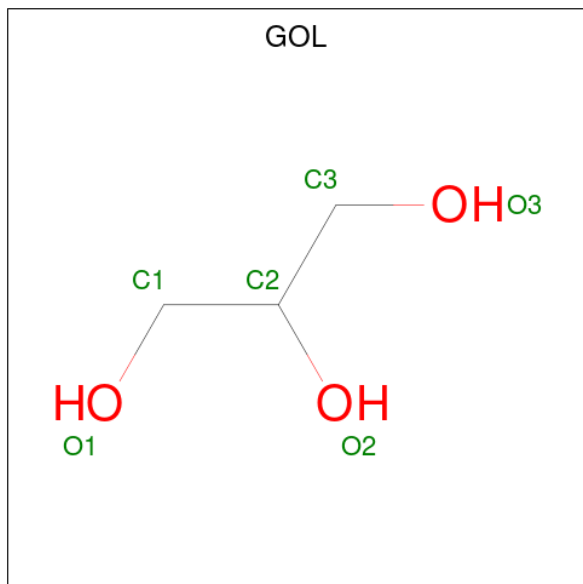
- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-methyl 2-thio-alpha-D-mannopyranoside.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	2	Total	C	O	S	0	0	0
			24	13	10	1			
2	H	2	Total	C	O	S	0	0	0
			24	13	10	1			
2	I	2	Total	C	O	S	0	0	0
			24	13	10	1			
2	J	2	Total	C	O	S	0	0	0
			24	13	10	1			
2	K	2	Total	C	O	S	0	0	0
			24	13	10	1			
2	L	2	Total	C	O	S	0	0	0
			24	13	10	1			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0

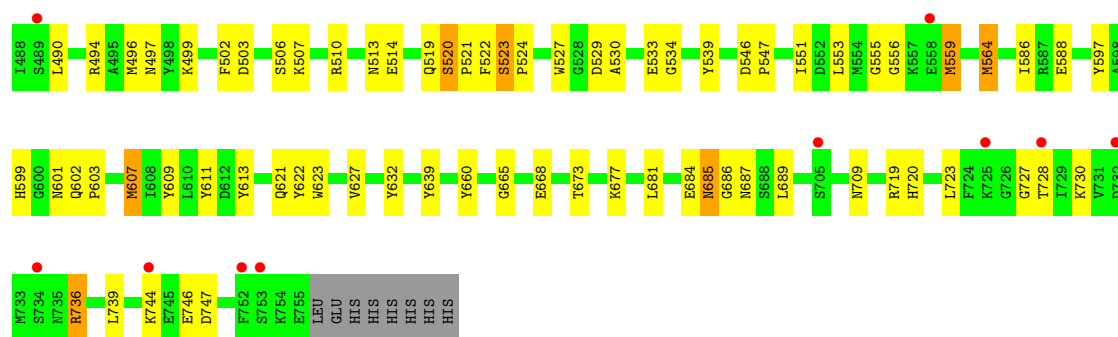
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	230	Total O 230 230	0	0

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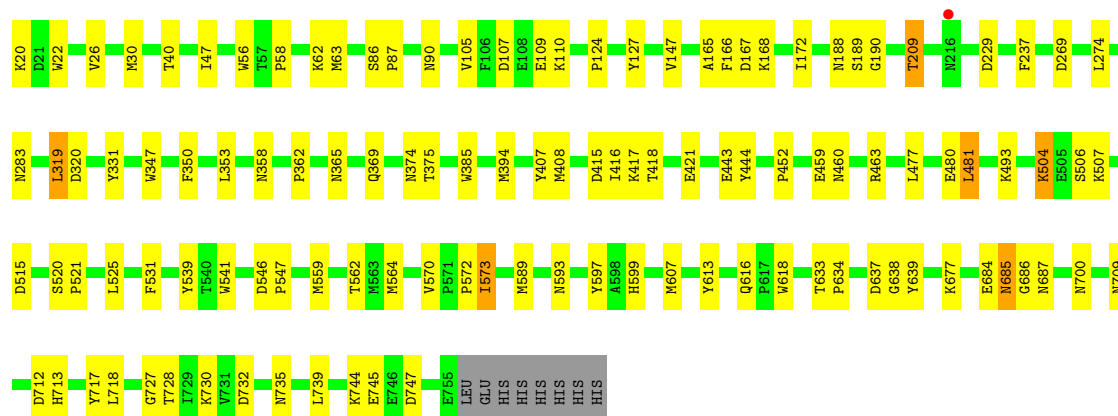
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	162	Total 162	O 162	0	0
5	C	322	Total 322	O 322	0	0
5	D	155	Total 155	O 155	0	0
5	E	217	Total 217	O 217	0	0
5	F	195	Total 195	O 195	0	0



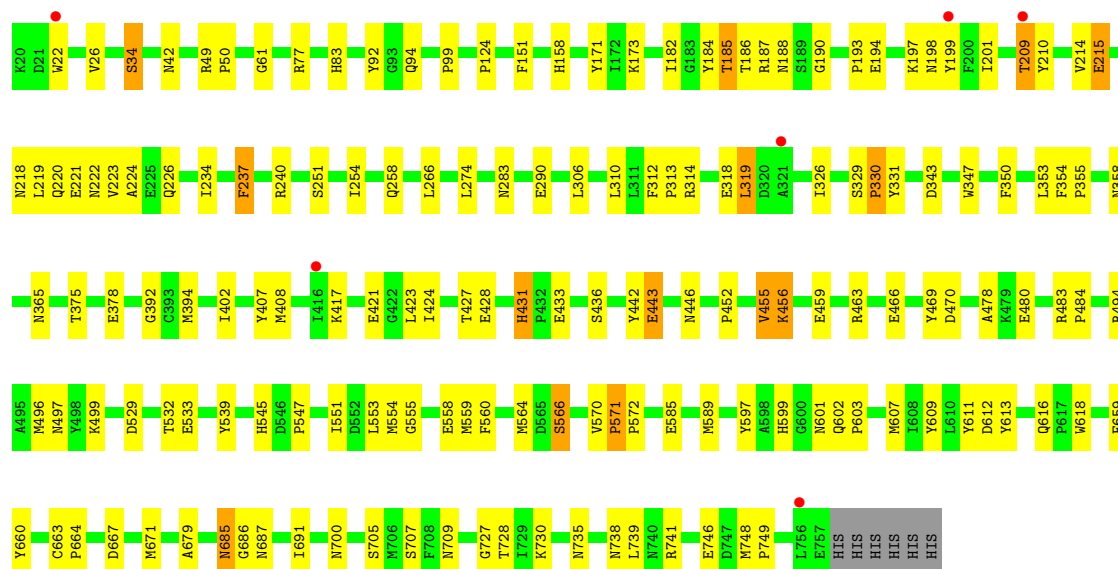
• Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE

Chain C: 83% 15% ..

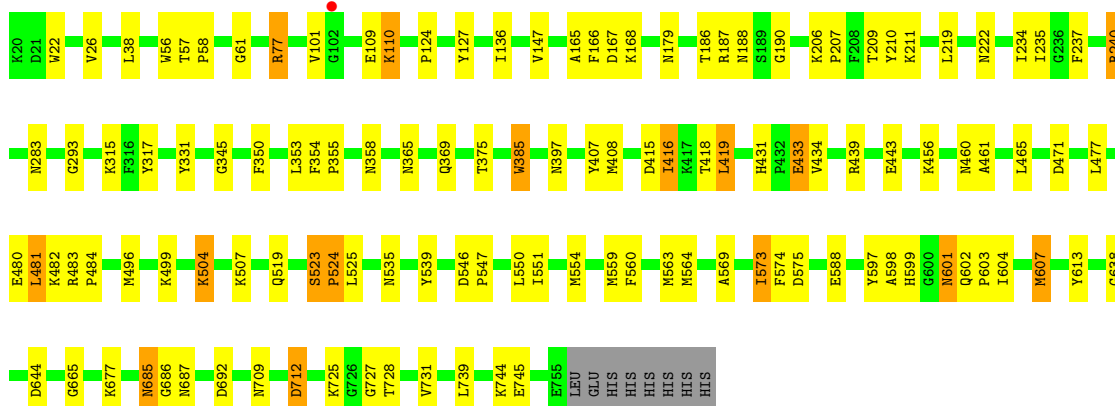


• Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE

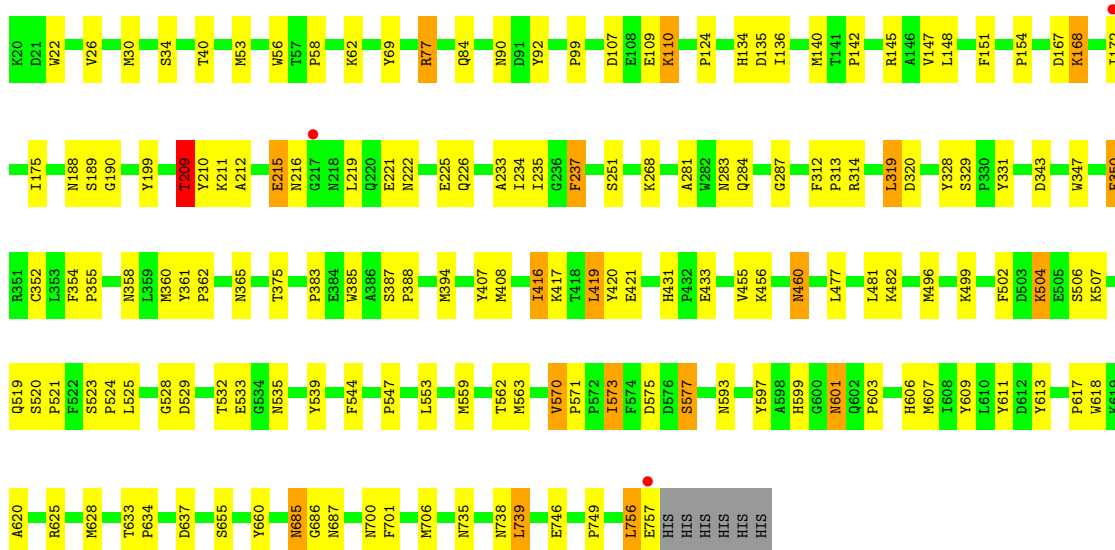
Chain D: 77% 20% ..



• Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE



Chain F: 78% 19% .



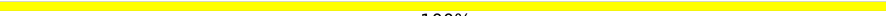
- Molecule 2: α -D-mannopyranose-(1-2)-methyl 2-thio- α -D-mannopyranoside



- Molecule 2: alpha-D-mannopyranose-(1-2)-methyl 2-thio-alpha-D-mannopyranoside

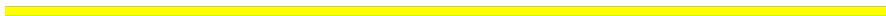


- Molecule 2: alpha-D-mannopyranose-(1-2)-methyl 2-thio-alpha-D-mannopyranoside

Chain I:  100%

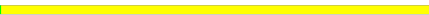
Z5L1
MAN2

- Molecule 2: alpha-D-mannopyranose-(1-2)-methyl 2-thio-alpha-D-mannopyranoside

Chain J:  100%

Z5L1
MAN2

- Molecule 2: alpha-D-mannopyranose-(1-2)-methyl 2-thio-alpha-D-mannopyranoside

Chain K:  50%  50%

Z5L1
MAN2

- Molecule 2: alpha-D-mannopyranose-(1-2)-methyl 2-thio-alpha-D-mannopyranoside

Chain L:  100%

Z5L1
MAN2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	161.26Å 68.59Å 204.01Å 90.00° 94.66° 90.00°	Depositor
Resolution (Å)	203.33 – 2.10 203.33 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.3 (203.33-2.10) 97.3 (203.33-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.190 , 0.244 0.195 , 0.249	Depositor DCC
R_{free} test set	12627 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	37131	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6577e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, CA, GOL, Z5L

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	0.65	0/6138	0.86	3/8330 (0.0%)
1	B	0.68	0/6118	0.90	11/8307 (0.1%)
1	C	0.67	0/6130	0.86	2/8320 (0.0%)
1	D	0.62	1/6127 (0.0%)	0.86	4/8324 (0.0%)
1	E	0.65	0/6129	0.88	11/8322 (0.1%)
1	F	0.57	0/6129	0.85	9/8323 (0.1%)
All	All	0.64	1/36771 (0.0%)	0.87	40/49926 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	571	PRO	C-O	-5.05	1.18	1.24

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	638	GLY	N-CA-C	7.65	121.91	112.73
1	E	523	SER	CA-C-N	7.35	126.99	119.56
1	E	523	SER	C-N-CA	7.35	126.99	119.56
1	B	447	LYS	N-CA-C	7.22	118.94	111.14
1	E	569	ALA	CA-C-N	-6.78	117.71	122.59
1	E	569	ALA	C-N-CA	-6.78	117.71	122.59
1	B	382	PHE	N-CA-C	-6.46	101.62	109.83
1	E	57	THR	CA-C-N	-6.43	113.15	119.78
1	E	57	THR	C-N-CA	-6.43	113.15	119.78
1	F	570	VAL	CB-CA-C	-6.07	104.21	110.71
1	B	523	SER	CA-C-N	5.95	125.57	119.56
1	B	523	SER	C-N-CA	5.95	125.57	119.56
1	A	638	GLY	N-CA-C	5.67	120.97	113.37
1	B	336	LEU	CA-C-N	5.63	125.56	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	336	LEU	C-N-CA	5.63	125.56	119.76
1	E	397	ASN	N-CA-C	-5.60	103.72	110.44
1	E	638	GLY	N-CA-C	5.60	120.87	113.37
1	F	570	VAL	N-CA-C	5.50	113.32	107.76
1	D	424	ILE	CB-CA-C	-5.50	104.93	111.97
1	B	249	ILE	N-CA-C	5.49	116.64	108.46
1	B	665	GLY	N-CA-C	-5.47	107.39	113.79
1	A	218	ASN	N-CA-C	5.45	117.61	108.73
1	A	402	ILE	CB-CA-C	-5.44	104.92	111.88
1	E	665	GLY	N-CA-C	-5.34	107.54	113.79
1	F	84	GLN	CA-C-N	5.34	126.52	119.84
1	F	84	GLN	C-N-CA	5.34	126.52	119.84
1	F	209	THR	N-CA-C	-5.30	106.84	113.72
1	D	330	PRO	N-CA-C	-5.29	107.85	114.20
1	B	443	GLU	N-CA-C	-5.23	105.47	111.07
1	F	328	TYR	N-CA-C	-5.21	102.67	110.23
1	F	460	ASN	N-CA-C	5.14	117.79	111.82
1	B	668	GLU	N-CA-C	5.09	117.78	109.59
1	E	524	PRO	N-CA-C	-5.09	107.50	113.86
1	F	523	SER	CA-C-N	5.09	124.88	119.28
1	F	523	SER	C-N-CA	5.09	124.88	119.28
1	B	556	GLY	N-CA-C	5.07	118.19	111.70
1	E	607	MET	N-CA-C	5.04	117.16	111.11
1	C	209	THR	N-CA-C	-5.04	107.81	114.31
1	D	431	HIS	CA-C-N	5.02	124.62	119.05
1	D	431	HIS	C-N-CA	5.02	124.62	119.05

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5957	0	5610	121	0
1	B	5937	0	5576	235	0
1	C	5949	0	5600	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	5946	0	5557	155	0
1	E	5945	0	5577	92	0
1	F	5948	0	5582	138	0
2	G	24	0	9	0	0
2	H	24	0	9	0	0
2	I	24	0	8	0	0
2	J	24	0	8	0	0
2	K	24	0	8	0	0
2	L	24	0	8	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	6	0	8	0	0
4	C	6	0	8	0	0
4	E	6	0	8	0	0
5	A	230	0	0	4	0
5	B	162	0	0	5	0
5	C	322	0	0	3	0
5	D	155	0	0	3	0
5	E	217	0	0	1	0
5	F	195	0	0	4	0
All	All	37131	0	33576	824	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (824) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:TYR:CZ	1:B:455:VAL:HG11	1.50	1.44
1:F:211:LYS:NZ	1:F:222:ASN:OD1	1.63	1.31
1:D:318:GLU:C	1:D:319:LEU:HD23	1.55	1.30
1:D:554:MET:O	1:D:559:MET:CE	1.81	1.26
1:B:446:ASN:HD21	1:B:494:ARG:NH1	1.39	1.21
1:B:446:ASN:ND2	1:B:494:ARG:NH1	1.88	1.20
1:A:496:MET:HA	1:A:496:MET:CE	1.73	1.18
1:A:407:TYR:HD1	1:A:408:MET:HE3	0.99	1.15
1:B:363:SER:OG	1:B:684:GLU:OE2	1.63	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:LEU:HD12	1:B:441:GLY:N	1.60	1.15
1:D:319:LEU:HD23	1:D:319:LEU:N	1.53	1.14
1:A:407:TYR:HD1	1:A:408:MET:CE	1.61	1.14
1:D:329:SER:OG	1:D:378:GLU:OE1	1.62	1.14
1:D:554:MET:O	1:D:559:MET:HE3	1.44	1.14
1:A:416:ILE:HD11	1:A:481:LEU:HD11	1.17	1.13
1:B:444:TYR:OH	1:B:455:VAL:CG1	1.96	1.12
1:B:482:LYS:NZ	1:B:482:LYS:HB2	1.58	1.11
1:A:416:ILE:CD1	1:A:481:LEU:HD11	1.81	1.10
1:F:496:MET:CE	1:F:499:LYS:HE3	1.80	1.10
1:B:444:TYR:OH	1:B:455:VAL:HG11	1.47	1.09
1:B:736:ARG:HH11	1:B:736:ARG:CG	1.63	1.09
1:B:482:LYS:HB2	1:B:482:LYS:HZ2	0.94	1.08
1:F:573:ILE:HD13	1:F:573:ILE:H	0.96	1.08
1:A:496:MET:HE3	1:A:496:MET:CA	1.79	1.08
1:A:408:MET:HE2	1:A:408:MET:HA	1.35	1.07
1:D:496:MET:CE	1:D:499:LYS:HE3	1.84	1.06
1:B:496:MET:HE2	1:B:499:LYS:HE3	1.13	1.06
1:A:601:ASN:HD22	1:A:603:PRO:HD2	1.18	1.05
1:B:490:LEU:HD11	1:B:494:ARG:HH21	1.20	1.04
1:A:407:TYR:CD1	1:A:408:MET:HE3	1.92	1.03
1:E:240:ARG:HH11	1:E:240:ARG:HG2	1.20	1.03
1:F:573:ILE:H	1:F:573:ILE:CD1	1.70	1.03
1:B:547:PRO:HG2	1:B:613:TYR:CE2	1.93	1.03
1:A:496:MET:HE2	1:A:499:LYS:CE	1.88	1.02
1:A:496:MET:HE2	1:A:499:LYS:HE3	1.02	1.02
1:B:496:MET:HE2	1:B:499:LYS:CE	1.90	1.01
1:C:407:TYR:HD1	1:C:408:MET:HE2	1.23	1.01
1:B:444:TYR:CZ	1:B:455:VAL:CG1	2.43	1.01
1:D:496:MET:HE1	1:D:499:LYS:HE3	1.38	1.00
1:B:452:PRO:HB2	1:B:455:VAL:HG22	1.43	1.00
1:F:601:ASN:ND2	1:F:603:PRO:HD2	1.74	1.00
1:A:157:ASP:HA	1:A:238:LYS:HG2	1.42	0.99
1:E:407:TYR:HD1	1:E:408:MET:CE	1.75	0.99
1:B:440:LEU:HD12	1:B:441:GLY:H	1.18	0.99
1:D:407:TYR:HD1	1:D:408:MET:HE2	1.27	0.99
1:A:407:TYR:CD1	1:A:408:MET:CE	2.45	0.98
1:B:188:ASN:HD22	1:B:190:GLY:H	1.09	0.97
1:A:601:ASN:ND2	1:A:603:PRO:HD2	1.79	0.97
1:B:319:LEU:N	1:B:319:LEU:HD22	1.74	0.97
1:A:496:MET:HE1	1:A:498:TYR:CE1	1.98	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:601:ASN:OD1	1:D:603:PRO:HD2	1.63	0.96
1:F:573:ILE:HD13	1:F:573:ILE:N	1.79	0.96
1:B:736:ARG:NH1	1:B:736:ARG:HG2	1.56	0.95
1:A:496:MET:CE	1:A:499:LYS:HE3	1.96	0.94
1:C:504:LYS:HG3	5:C:2216:HOH:O	1.66	0.94
1:B:482:LYS:NZ	1:B:482:LYS:CB	2.30	0.92
1:B:736:ARG:HH11	1:B:736:ARG:HG2	0.77	0.92
1:B:446:ASN:HD21	1:B:494:ARG:HH11	0.97	0.92
1:B:157:ASP:OD1	1:B:238:LYS:HE3	1.70	0.92
1:A:416:ILE:HD11	1:A:481:LEU:CD1	2.00	0.92
1:F:525:LEU:HD13	1:F:573:ILE:HG12	1.52	0.91
1:D:215:GLU:HB2	1:D:226:GLN:NE2	1.87	0.90
1:F:219:LEU:HD11	1:F:234:ILE:HD12	1.55	0.89
1:C:407:TYR:HD1	1:C:408:MET:CE	1.84	0.89
1:A:248:ARG:NH2	1:A:267:GLY:O	2.05	0.89
1:B:685:ASN:ND2	1:B:687:ASN:H	1.71	0.88
1:D:496:MET:CE	1:D:499:LYS:CE	2.51	0.88
1:B:431:HIS:HD2	1:B:434:VAL:H	1.17	0.88
1:E:507:LYS:HE3	1:E:559:MET:HE2	1.54	0.87
1:D:319:LEU:N	1:D:319:LEU:CD2	2.34	0.87
1:E:240:ARG:HG2	1:E:240:ARG:NH1	1.85	0.87
1:A:188:ASN:HD22	1:A:190:GLY:H	1.22	0.86
1:C:559:MET:HE3	1:C:562:THR:HB	1.54	0.86
5:A:2213:HOH:O	1:D:158:HIS:CE1	2.28	0.86
1:B:407:TYR:CE2	1:B:416:ILE:CD1	2.58	0.86
1:F:419:LEU:HD12	1:F:419:LEU:O	1.75	0.86
1:B:744:LYS:HE2	1:B:747:ASP:OD2	1.76	0.86
1:F:375:THR:HG21	1:F:383:PRO:HD3	1.57	0.86
1:B:444:TYR:OH	1:B:455:VAL:HG12	1.75	0.85
1:F:419:LEU:HD12	1:F:419:LEU:C	2.02	0.85
1:D:407:TYR:CD1	1:D:408:MET:HE2	2.12	0.85
1:D:188:ASN:HD22	1:D:190:GLY:H	1.21	0.85
1:D:318:GLU:C	1:D:319:LEU:CD2	2.47	0.85
1:E:407:TYR:HD1	1:E:408:MET:HE2	1.37	0.84
1:B:496:MET:CE	1:B:499:LYS:HE3	2.04	0.84
1:A:525:LEU:HD13	1:A:573:ILE:HG12	1.59	0.84
1:F:570:VAL:O	1:F:570:VAL:HG23	1.74	0.84
1:E:219:LEU:HD11	1:E:234:ILE:HD12	1.60	0.83
1:B:506:SER:O	1:B:507:LYS:HB2	1.76	0.83
1:D:22:TRP:H	1:D:283:ASN:HD21	1.26	0.83
1:C:416:ILE:HD11	1:C:481:LEU:HD11	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:ASN:HD22	1:C:190:GLY:H	1.26	0.83
1:F:496:MET:HE1	1:F:499:LYS:HE3	1.60	0.83
1:B:685:ASN:C	1:B:685:ASN:HD22	1.84	0.83
1:C:358:ASN:HD21	1:C:365:ASN:HD22	1.21	0.82
1:B:407:TYR:HE2	1:B:416:ILE:HD12	1.44	0.82
1:A:358:ASN:HD21	1:A:365:ASN:HD22	1.24	0.81
1:E:407:TYR:CD1	1:E:408:MET:CE	2.63	0.81
1:B:446:ASN:CG	1:B:494:ARG:NH1	2.38	0.81
1:D:555:GLY:HA3	1:D:559:MET:CE	2.10	0.81
1:D:358:ASN:HD21	1:D:365:ASN:HD22	1.29	0.81
1:E:188:ASN:HD22	1:E:190:GLY:H	1.28	0.81
1:E:358:ASN:HD21	1:E:365:ASN:HD22	1.27	0.81
1:F:358:ASN:ND2	1:F:365:ASN:HD22	1.78	0.80
1:B:319:LEU:N	1:B:319:LEU:CD2	2.44	0.80
1:B:407:TYR:HE2	1:B:416:ILE:CD1	1.94	0.80
1:F:496:MET:CE	1:F:499:LYS:CE	2.60	0.80
1:B:193:PRO:HD3	1:B:330:PRO:O	1.82	0.80
1:F:571:PRO:O	1:F:573:ILE:CD1	2.30	0.80
1:B:22:TRP:H	1:B:283:ASN:HD21	1.26	0.80
1:B:445:TYR:OH	1:B:471:ASP:OD2	2.00	0.80
1:D:685:ASN:C	1:D:685:ASN:HD22	1.89	0.80
1:D:331:TYR:CZ	1:D:375:THR:HG23	2.16	0.79
1:A:496:MET:HA	1:A:496:MET:HE3	0.87	0.79
1:C:417:LYS:O	1:C:421:GLU:HG3	1.81	0.79
1:D:215:GLU:HB2	1:D:226:GLN:HE21	1.46	0.79
1:E:416:ILE:HG12	1:E:416:ILE:O	1.82	0.79
1:B:490:LEU:HD11	1:B:494:ARG:NH2	1.96	0.79
1:B:564:MET:HE2	1:B:611:TYR:CZ	2.18	0.79
1:B:449:GLY:HA2	1:B:497:ASN:HD21	1.46	0.79
1:E:477:LEU:HG	1:E:481:LEU:HD22	1.64	0.79
1:F:407:TYR:HD1	1:F:408:MET:HE2	1.46	0.79
1:F:22:TRP:H	1:F:283:ASN:ND2	1.80	0.78
1:F:575:ASP:OD1	1:F:577:SER:OG	2.01	0.78
1:E:550:LEU:HD11	1:E:554:MET:CE	2.14	0.78
1:B:407:TYR:CE2	1:B:416:ILE:HD11	2.19	0.77
1:B:431:HIS:CD2	1:B:433:GLU:H	2.02	0.77
1:F:571:PRO:O	1:F:573:ILE:HD13	1.84	0.77
1:C:407:TYR:CD1	1:C:408:MET:CE	2.66	0.77
1:E:240:ARG:HH11	1:E:240:ARG:CG	1.97	0.77
1:B:376:TYR:HE1	1:B:380:GLY:O	1.67	0.77
1:E:550:LEU:CG	1:E:554:MET:HE3	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ASN:ND2	1:B:190:GLY:H	1.83	0.76
1:B:446:ASN:CG	1:B:494:ARG:HH12	1.92	0.76
1:B:496:MET:CE	1:B:499:LYS:CE	2.63	0.76
1:D:331:TYR:CE2	1:D:375:THR:HG23	2.21	0.76
1:F:172:ILE:HD13	1:F:233:ALA:HB2	1.66	0.76
1:C:358:ASN:ND2	1:C:365:ASN:HD22	1.84	0.76
1:B:431:HIS:CD2	1:B:434:VAL:H	2.02	0.76
1:F:685:ASN:HD22	1:F:685:ASN:C	1.94	0.76
1:F:22:TRP:H	1:F:283:ASN:HD21	1.34	0.75
1:C:744:LYS:HE2	1:C:747:ASP:OD2	1.86	0.74
1:E:550:LEU:HG	1:E:554:MET:HE3	1.68	0.74
1:D:358:ASN:ND2	1:D:365:ASN:HD22	1.84	0.74
1:A:408:MET:HE2	1:A:408:MET:CA	2.13	0.74
1:C:22:TRP:H	1:C:283:ASN:ND2	1.84	0.74
1:E:685:ASN:C	1:E:685:ASN:HD22	1.94	0.74
1:A:571:PRO:O	1:A:573:ILE:HD13	1.86	0.74
1:E:550:LEU:CD1	1:E:554:MET:HE3	2.17	0.74
1:B:440:LEU:HD12	1:B:440:LEU:C	2.10	0.74
1:D:555:GLY:HA3	1:D:559:MET:HE1	1.70	0.73
1:B:376:TYR:CE1	1:B:380:GLY:O	2.41	0.73
1:B:363:SER:OG	1:B:684:GLU:CD	2.32	0.73
1:C:415:ASP:OD2	1:C:418:THR:OG1	2.07	0.73
1:E:550:LEU:HD11	1:E:554:MET:HE3	1.70	0.73
1:B:454:ASP:OD2	1:B:513:ASN:HB3	1.88	0.73
1:F:496:MET:HE2	1:F:499:LYS:NZ	2.04	0.73
1:B:358:ASN:HD21	1:B:365:ASN:HD22	1.35	0.73
1:D:554:MET:O	1:D:559:MET:HE2	1.87	0.73
1:A:408:MET:CE	1:A:408:MET:HA	2.18	0.72
1:F:431:HIS:HD2	1:F:433:GLU:H	1.37	0.72
1:B:506:SER:O	1:B:507:LYS:CB	2.38	0.72
1:F:375:THR:CG2	1:F:383:PRO:HD3	2.19	0.72
1:A:559:MET:HE3	1:A:562:THR:HB	1.71	0.72
1:A:685:ASN:ND2	1:A:687:ASN:H	1.87	0.72
1:B:97:ILE:HD11	1:B:161:VAL:HG11	1.72	0.72
1:A:358:ASN:ND2	1:A:365:ASN:HD22	1.87	0.72
1:A:496:MET:CE	1:A:498:TYR:CE1	2.72	0.72
1:B:415:ASP:OD2	1:B:418:THR:OG1	2.08	0.72
1:A:525:LEU:HD13	1:A:573:ILE:CG1	2.20	0.71
1:C:22:TRP:H	1:C:283:ASN:HD21	1.35	0.71
1:F:416:ILE:HD11	1:F:481:LEU:HD21	1.72	0.71
1:B:347:TRP:CZ3	1:B:394:MET:HE2	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:ILE:HD13	1:D:326:ILE:HD12	1.73	0.71
1:F:685:ASN:HD22	1:F:686:GLY:N	1.89	0.71
1:B:22:TRP:H	1:B:283:ASN:ND2	1.89	0.70
1:A:417:LYS:O	1:A:421:GLU:HG3	1.90	0.70
1:F:188:ASN:HD22	1:F:190:GLY:H	1.38	0.70
1:F:358:ASN:HD21	1:F:365:ASN:HD22	1.38	0.70
1:B:407:TYR:HD1	1:B:408:MET:HE2	1.57	0.70
1:D:22:TRP:H	1:D:283:ASN:ND2	1.89	0.70
1:D:483:ARG:HB3	1:D:484:PRO:HD2	1.74	0.70
1:F:496:MET:HE2	1:F:499:LYS:CE	2.22	0.69
1:E:22:TRP:H	1:E:283:ASN:ND2	1.90	0.69
1:A:496:MET:CE	1:A:496:MET:CA	2.50	0.69
1:C:547:PRO:HG2	1:C:613:TYR:CE2	2.28	0.69
1:F:235:ILE:O	1:F:235:ILE:HD12	1.93	0.69
1:B:158:HIS:NE2	5:B:2059:HOH:O	2.21	0.69
1:F:507:LYS:HE3	1:F:559:MET:SD	2.33	0.69
1:B:377:LEU:HD21	1:B:418:THR:HG21	1.74	0.69
1:F:30:MET:HE3	1:F:633:THR:O	1.92	0.68
1:B:744:LYS:CE	1:B:747:ASP:OD2	2.42	0.68
1:D:685:ASN:ND2	1:D:687:ASN:H	1.91	0.68
1:A:559:MET:HE3	1:A:559:MET:O	1.93	0.68
1:B:327:HIS:ND1	1:B:338:GLY:O	2.27	0.68
1:C:408:MET:HE1	1:C:480:GLU:HG2	1.76	0.67
1:D:459:GLU:O	1:D:463:ARG:HG3	1.95	0.67
1:A:597:TYR:OH	1:A:599:HIS:HD2	1.76	0.67
1:B:174:ILE:O	1:B:176:PRO:HD3	1.95	0.67
1:F:319:LEU:HD22	1:F:319:LEU:N	2.09	0.67
1:B:407:TYR:CE2	1:B:416:ILE:HD12	2.26	0.67
1:B:685:ASN:HD22	1:B:686:GLY:N	1.92	0.67
1:C:407:TYR:CD1	1:C:408:MET:HE2	2.16	0.67
1:C:477:LEU:HG	1:C:481:LEU:HD22	1.76	0.67
1:F:685:ASN:ND2	1:F:687:ASN:H	1.94	0.66
1:C:407:TYR:CE2	1:C:416:ILE:HD12	2.30	0.66
1:B:358:ASN:ND2	1:B:365:ASN:HD22	1.93	0.66
1:B:450:TYR:OH	1:B:513:ASN:O	2.09	0.66
1:E:685:ASN:ND2	1:E:687:ASN:H	1.94	0.66
1:B:454:ASP:OD2	1:B:513:ASN:CA	2.44	0.66
1:B:454:ASP:OD2	1:B:513:ASN:CB	2.44	0.66
1:A:431:HIS:CD2	1:A:433:GLU:H	2.14	0.66
1:D:221:GLU:O	1:D:222:ASN:HB2	1.96	0.66
1:E:709:ASN:HD21	1:E:727:GLY:HA3	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:559:MET:CE	1:C:562:THR:HB	2.26	0.65
1:F:431:HIS:CD2	1:F:433:GLU:H	2.14	0.65
1:A:547:PRO:HG2	1:A:613:TYR:CE2	2.31	0.65
5:A:2213:HOH:O	1:D:158:HIS:HE1	1.69	0.65
1:B:454:ASP:OD2	1:B:513:ASN:HA	1.96	0.65
1:B:419:LEU:O	1:B:419:LEU:HD12	1.97	0.65
1:C:331:TYR:CZ	1:C:375:THR:HG23	2.31	0.65
1:B:347:TRP:CE3	1:B:394:MET:HE2	2.32	0.65
1:B:483:ARG:NE	1:B:487:GLU:OE2	2.30	0.65
1:A:628:MET:HE2	1:A:655:SER:HB3	1.78	0.65
1:B:685:ASN:HD22	1:B:687:ASN:H	1.45	0.65
1:E:22:TRP:H	1:E:283:ASN:HD21	1.45	0.64
1:A:477:LEU:HG	1:A:481:LEU:HD22	1.80	0.64
1:B:459:GLU:O	1:B:463:ARG:HG3	1.96	0.64
1:B:483:ARG:NH2	1:B:487:GLU:OE2	2.30	0.64
1:E:431:HIS:HD2	1:E:433:GLU:H	1.42	0.64
1:B:431:HIS:HD2	1:B:434:VAL:N	1.94	0.64
1:B:744:LYS:HE2	1:B:747:ASP:CG	2.21	0.64
1:D:215:GLU:CB	1:D:226:GLN:NE2	2.61	0.64
1:D:318:GLU:O	1:D:319:LEU:HD23	1.98	0.64
1:D:709:ASN:ND2	1:D:728:THR:H	1.95	0.64
1:B:384:GLU:OE2	1:B:399:SER:OG	2.13	0.64
1:B:483:ARG:HH21	1:B:487:GLU:CD	2.06	0.64
1:D:555:GLY:HA3	1:D:559:MET:HE2	1.77	0.63
1:E:601:ASN:ND2	1:E:603:PRO:HD2	2.12	0.63
1:B:335:VAL:HG23	5:B:2105:HOH:O	1.98	0.63
1:B:440:LEU:CD1	1:B:441:GLY:N	2.51	0.63
1:C:62:LYS:NZ	1:C:109:GLU:CD	2.55	0.63
1:C:506:SER:O	1:C:507:LYS:HB2	1.97	0.63
1:D:564:MET:HE2	1:D:611:TYR:CZ	2.33	0.63
1:D:555:GLY:CA	1:D:559:MET:HE2	2.28	0.63
1:A:496:MET:HE1	1:A:498:TYR:HE1	1.61	0.63
1:C:347:TRP:CZ3	1:C:394:MET:HE2	2.33	0.63
1:B:425:HIS:O	1:B:425:HIS:ND1	2.32	0.62
1:A:22:TRP:H	1:A:283:ASN:HD21	1.47	0.62
1:B:483:ARG:NH2	1:B:487:GLU:CD	2.58	0.62
1:B:483:ARG:CZ	1:B:487:GLU:OE2	2.47	0.62
1:C:745:GLU:OE1	1:C:745:GLU:C	2.42	0.62
1:A:22:TRP:H	1:A:283:ASN:ND2	1.97	0.62
1:A:407:TYR:CD1	1:A:408:MET:HE1	2.33	0.62
1:A:573:ILE:HD13	1:A:573:ILE:H	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:HIS:ND1	1:B:425:HIS:C	2.57	0.62
1:B:449:GLY:HA2	1:B:497:ASN:ND2	2.14	0.62
1:D:22:TRP:CZ2	1:D:290:GLU:HG2	2.35	0.62
1:D:496:MET:HE2	1:D:499:LYS:NZ	2.14	0.62
1:B:444:TYR:CE1	1:B:455:VAL:HG11	2.24	0.62
1:C:685:ASN:ND2	1:C:687:ASN:H	1.97	0.62
1:E:358:ASN:ND2	1:E:365:ASN:HD22	1.97	0.62
1:A:431:HIS:HD2	1:A:433:GLU:H	1.47	0.61
1:F:26:VAL:HG11	1:F:124:PRO:HG3	1.82	0.61
1:B:443:GLU:OE1	1:B:443:GLU:N	2.30	0.61
1:E:597:TYR:OH	1:E:599:HIS:HD2	1.83	0.61
1:F:235:ILE:HD12	1:F:235:ILE:C	2.25	0.61
1:B:496:MET:HE3	1:B:496:MET:HA	1.81	0.61
1:A:62:LYS:HE2	1:A:109:GLU:OE1	2.00	0.61
1:B:685:ASN:ND2	1:B:685:ASN:C	2.53	0.61
1:D:564:MET:HE3	1:D:607:MET:HE3	1.81	0.61
1:B:444:TYR:HH	1:B:455:VAL:CG1	2.12	0.61
1:F:573:ILE:CD1	1:F:573:ILE:N	2.48	0.61
1:B:547:PRO:HB2	1:B:613:TYR:CD2	2.36	0.61
1:B:431:HIS:HD2	1:B:433:GLU:H	1.44	0.61
1:F:597:TYR:OH	1:F:599:HIS:HD2	1.83	0.61
1:A:685:ASN:HD22	1:A:685:ASN:C	2.09	0.60
1:D:354:PHE:CD2	1:D:402:ILE:HD12	2.36	0.60
1:F:347:TRP:CZ3	1:F:394:MET:HE2	2.36	0.60
1:C:573:ILE:HD13	1:C:573:ILE:H	1.66	0.60
1:E:431:HIS:CD2	1:E:433:GLU:H	2.19	0.60
1:A:416:ILE:CD1	1:A:481:LEU:CD1	2.69	0.60
1:B:474:ILE:O	1:B:475:TYR:C	2.44	0.60
1:B:482:LYS:CB	1:B:482:LYS:HZ3	2.14	0.60
1:D:331:TYR:CZ	1:D:375:THR:CG2	2.84	0.60
1:C:685:ASN:C	1:C:685:ASN:HD22	2.07	0.60
1:B:318:GLU:C	1:B:319:LEU:HD22	2.26	0.60
1:E:61:GLY:O	1:E:77:ARG:HD3	2.01	0.60
1:E:407:TYR:CD1	1:E:408:MET:HE2	2.29	0.60
1:C:459:GLU:O	1:C:463:ARG:HG3	2.02	0.59
1:C:362:PRO:HD2	1:C:684:GLU:CD	2.27	0.59
1:F:314:ARG:NE	1:F:343:ASP:OD2	2.31	0.59
1:B:199:TYR:O	1:B:251:SER:HA	2.03	0.59
1:D:171:TYR:HB3	1:D:184:TYR:CE2	2.37	0.59
1:D:496:MET:HE1	1:D:499:LYS:CE	2.21	0.59
1:E:407:TYR:CD1	1:E:408:MET:HE1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:PRO:HG3	1:E:127:TYR:CZ	2.37	0.59
1:B:407:TYR:CD1	1:B:408:MET:HE2	2.35	0.59
1:C:685:ASN:HD22	1:C:686:GLY:N	2.01	0.59
1:E:525:LEU:HD13	1:E:573:ILE:HG23	1.82	0.59
1:A:504:LYS:HG3	5:A:2140:HOH:O	2.02	0.59
1:B:444:TYR:CE2	1:B:455:VAL:HG11	2.28	0.59
1:B:685:ASN:HD21	1:B:687:ASN:HB2	1.67	0.59
1:F:188:ASN:ND2	1:F:190:GLY:H	2.00	0.59
1:D:709:ASN:HD21	1:D:728:THR:H	1.50	0.58
1:F:62:LYS:NZ	1:F:109:GLU:OE2	2.34	0.58
1:E:564:MET:HE3	1:E:607:MET:HG2	1.85	0.58
1:A:347:TRP:CZ3	1:A:394:MET:HE2	2.37	0.58
1:D:483:ARG:HB3	1:D:484:PRO:CD	2.33	0.58
1:C:709:ASN:HD21	1:C:728:THR:H	1.50	0.58
1:B:547:PRO:O	1:B:551:ILE:HG13	2.04	0.58
1:D:685:ASN:C	1:D:685:ASN:ND2	2.58	0.58
1:B:235:ILE:HD12	1:B:235:ILE:C	2.29	0.58
1:C:597:TYR:OH	1:C:599:HIS:HD2	1.86	0.58
1:E:712:ASP:OD2	5:E:2202:HOH:O	2.17	0.58
1:F:613:TYR:CE2	1:F:749:PRO:HB2	2.39	0.58
1:A:506:SER:O	1:A:507:LYS:HB2	2.04	0.57
1:F:617:PRO:HD2	1:F:618:TRP:CE3	2.39	0.57
1:A:559:MET:HE2	1:A:563:MET:HG2	1.87	0.57
1:C:709:ASN:ND2	1:C:728:THR:H	2.03	0.57
1:D:431:HIS:HD2	1:D:433:GLU:H	1.52	0.57
1:B:490:LEU:CD1	1:B:494:ARG:HH21	2.07	0.57
1:F:533:GLU:O	1:F:601:ASN:OD1	2.22	0.57
1:B:602:GLN:N	1:B:603:PRO:CD	2.68	0.57
1:A:431:HIS:CD2	1:A:434:VAL:H	2.23	0.57
1:C:26:VAL:HG11	1:C:124:PRO:HG3	1.87	0.57
1:F:350:PHE:C	1:F:350:PHE:CD2	2.82	0.57
1:B:477:LEU:CD1	1:B:481:LEU:HD11	2.35	0.57
1:C:525:LEU:HD13	1:C:573:ILE:HG12	1.87	0.57
1:A:709:ASN:HD21	1:A:727:GLY:HA3	1.69	0.57
1:D:597:TYR:OH	1:D:599:HIS:HD2	1.87	0.57
1:E:110:LYS:HD2	1:E:110:LYS:N	2.13	0.57
1:A:188:ASN:ND2	1:A:190:GLY:H	2.00	0.56
1:D:431:HIS:CD2	1:D:433:GLU:H	2.23	0.56
1:C:365:ASN:O	1:C:369:GLN:HG2	2.05	0.56
1:B:519:GLN:HB2	5:B:2120:HOH:O	2.05	0.56
1:B:736:ARG:CG	1:B:736:ARG:NH1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:455:VAL:O	1:D:456:LYS:HB2	2.05	0.56
1:C:353:LEU:HD13	1:C:353:LEU:C	2.31	0.56
1:D:547:PRO:HG2	1:D:613:TYR:CE2	2.41	0.56
1:B:165:ALA:O	1:B:166:PHE:HB2	2.06	0.56
1:B:425:HIS:C	1:B:425:HIS:HD1	2.14	0.56
1:B:354:PHE:N	1:B:355:PRO:CD	2.69	0.56
1:E:685:ASN:HD22	1:E:686:GLY:N	2.04	0.56
1:A:709:ASN:ND2	1:A:728:THR:H	2.04	0.56
1:B:215:GLU:O	1:B:218:ASN:HB2	2.05	0.56
1:A:353:LEU:HD13	1:A:353:LEU:C	2.31	0.55
1:A:366:LYS:HE2	1:A:412:LYS:O	2.07	0.55
1:F:407:TYR:CD1	1:F:408:MET:HE2	2.36	0.55
1:B:194:GLU:HG2	1:E:725:LYS:HG2	1.87	0.55
1:C:58:PRO:HG3	1:C:127:TYR:CZ	2.41	0.55
1:E:601:ASN:ND2	1:E:601:ASN:C	2.64	0.55
1:A:520:SER:HA	1:A:521:PRO:C	2.30	0.55
1:F:570:VAL:O	1:F:570:VAL:CG2	2.49	0.55
1:E:483:ARG:HB3	1:E:484:PRO:HD2	1.87	0.55
1:F:361:TYR:N	1:F:362:PRO:CD	2.69	0.55
1:D:171:TYR:CB	1:D:184:TYR:CE2	2.89	0.55
1:F:90:ASN:HB3	1:F:189:SER:OG	2.07	0.55
1:B:405:ASP:OD1	1:B:409:LYS:NZ	2.37	0.55
1:A:496:MET:HE1	1:A:498:TYR:CZ	2.39	0.54
1:D:209:THR:CG2	1:D:209:THR:O	2.55	0.54
1:D:554:MET:O	1:D:559:MET:HE1	1.94	0.54
1:A:30:MET:HE3	1:A:633:THR:O	2.07	0.54
1:A:157:ASP:HA	1:A:238:LYS:CG	2.26	0.54
1:E:507:LYS:HB2	1:E:563:MET:HE2	1.89	0.54
1:F:209:THR:CG2	1:F:237:PHE:HA	2.38	0.54
1:F:358:ASN:HD21	1:F:365:ASN:ND2	2.04	0.54
1:D:407:TYR:CD1	1:D:408:MET:CE	2.86	0.54
1:D:452:PRO:HB2	1:D:455:VAL:HG22	1.89	0.54
1:F:559:MET:HE3	1:F:562:THR:HB	1.89	0.54
1:A:86:SER:HB2	1:A:87:PRO:HD2	1.90	0.54
1:B:331:TYR:CE2	1:B:375:THR:HG23	2.43	0.54
1:B:449:GLY:C	1:B:497:ASN:ND2	2.66	0.54
1:C:20:LYS:N	5:C:2001:HOH:O	2.41	0.54
1:B:564:MET:HE2	1:B:611:TYR:CE2	2.42	0.54
1:D:417:LYS:O	1:D:421:GLU:HG3	2.08	0.54
1:E:235:ILE:HD12	1:E:235:ILE:C	2.32	0.54
1:B:496:MET:HE3	1:B:499:LYS:HD2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:709:ASN:ND2	1:E:728:THR:H	2.06	0.54
1:A:97:ILE:HD11	1:A:161:VAL:HG11	1.91	0.53
1:D:347:TRP:CE3	1:D:394:MET:HE2	2.43	0.53
1:D:478:ALA:O	1:D:483:ARG:HG2	2.09	0.53
1:D:496:MET:CE	1:D:499:LYS:NZ	2.71	0.53
1:E:211:LYS:NZ	1:E:222:ASN:OD1	2.40	0.53
1:F:628:MET:HE2	1:F:655:SER:HB3	1.89	0.53
1:B:158:HIS:CE1	5:B:2059:HOH:O	2.62	0.53
1:B:477:LEU:O	1:B:481:LEU:HD13	2.09	0.53
1:B:621:GLN:HG2	1:B:673:THR:HB	1.89	0.53
1:D:219:LEU:HD11	1:D:234:ILE:HD12	1.91	0.53
1:B:185:THR:HG23	1:B:198:ASN:HB3	1.90	0.53
1:B:744:LYS:NZ	1:B:747:ASP:OD2	2.42	0.53
1:D:193:PRO:HD3	1:D:330:PRO:O	2.08	0.53
1:F:58:PRO:HG2	1:F:69:TYR:CD1	2.44	0.53
1:D:220:GLN:HA	1:D:220:GLN:OE1	2.09	0.53
1:A:416:ILE:HD11	1:A:481:LEU:HD21	1.91	0.53
1:A:211:LYS:NZ	1:A:222:ASN:OD1	2.35	0.52
1:A:685:ASN:HD22	1:A:686:GLY:N	2.07	0.52
1:B:382:PHE:CE2	1:B:403:LEU:HD13	2.44	0.52
1:D:358:ASN:HD21	1:D:365:ASN:ND2	2.03	0.52
1:A:173:LYS:HB2	1:A:225:GLU:HG3	1.91	0.52
1:B:430:VAL:HG21	1:B:440:LEU:HA	1.91	0.52
1:B:449:GLY:O	1:B:497:ASN:ND2	2.43	0.52
1:D:685:ASN:HD22	1:D:686:GLY:N	2.08	0.52
1:C:62:LYS:HZ1	1:C:109:GLU:CD	2.16	0.52
1:C:347:TRP:CE3	1:C:394:MET:HE2	2.45	0.52
1:D:171:TYR:HB3	1:D:184:TYR:CD2	2.45	0.52
1:D:185:THR:HG23	1:D:198:ASN:HB3	1.90	0.52
1:F:22:TRP:CZ3	1:F:287:GLY:HA3	2.45	0.52
1:F:107:ASP:HB3	1:F:110:LYS:HB2	1.91	0.52
1:A:431:HIS:HD2	1:A:434:VAL:H	1.57	0.52
1:D:572:PRO:HB2	1:D:589:MET:HE3	1.91	0.52
1:B:564:MET:CE	1:B:611:TYR:CE2	2.93	0.52
1:D:199:TYR:O	1:D:251:SER:HA	2.09	0.52
1:F:525:LEU:HD13	1:F:573:ILE:CG1	2.34	0.52
1:B:490:LEU:O	1:B:494:ARG:HG3	2.09	0.51
1:F:77:ARG:HH21	1:F:109:GLU:HA	1.74	0.51
1:B:503:ASP:C	1:B:503:ASP:OD1	2.53	0.51
1:F:685:ASN:C	1:F:685:ASN:ND2	2.63	0.51
1:F:394:MET:HE1	1:F:533:GLU:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:LEU:HD12	1:B:481:LEU:CD1	2.40	0.51
1:C:713:HIS:HE1	1:C:717:TYR:O	1.93	0.51
1:A:408:MET:CE	1:A:408:MET:CA	2.85	0.51
1:C:745:GLU:C	1:C:745:GLU:CD	2.78	0.51
1:D:609:TYR:CZ	1:D:660:TYR:HB2	2.46	0.51
1:B:408:MET:HE1	1:B:480:GLU:HG2	1.93	0.51
1:E:186:THR:O	1:E:187:ARG:C	2.53	0.51
1:A:496:MET:CE	1:A:499:LYS:CE	2.72	0.51
1:F:56:TRP:CE2	1:F:147:VAL:HG11	2.46	0.51
1:B:345:GLY:HA3	1:B:385:TRP:CE2	2.45	0.51
1:F:215:GLU:O	1:F:216:ASN:C	2.53	0.51
1:C:570:VAL:O	1:C:570:VAL:HG23	2.09	0.50
1:D:394:MET:HE1	1:D:532:THR:CG2	2.41	0.50
1:D:496:MET:HE3	1:D:499:LYS:HE3	1.84	0.50
1:B:419:LEU:HD12	1:B:419:LEU:C	2.33	0.50
1:C:63:MET:HG3	1:C:166:PHE:CE2	2.46	0.50
1:D:394:MET:HE3	1:D:532:THR:HG21	1.92	0.50
1:B:400:ALA:O	1:B:404:VAL:HG23	2.12	0.50
1:D:499:LYS:HE2	5:D:2109:HOH:O	2.10	0.50
1:E:602:GLN:NE2	1:E:644:ASP:OD2	2.41	0.50
1:F:53:MET:HB3	1:F:145:ARG:HG2	1.93	0.50
1:F:394:MET:HE1	1:F:533:GLU:CG	2.41	0.50
1:F:419:LEU:C	1:F:419:LEU:CD1	2.74	0.50
1:A:331:TYR:CE2	1:A:375:THR:HG23	2.47	0.50
1:B:381:PHE:CE2	1:B:425:HIS:HE1	2.29	0.50
1:C:700:ASN:HD22	1:C:735:ASN:HB3	1.76	0.50
1:E:419:LEU:HD12	1:E:419:LEU:C	2.37	0.50
1:F:22:TRP:N	1:F:283:ASN:HD21	2.04	0.50
1:E:685:ASN:C	1:E:685:ASN:ND2	2.61	0.50
1:F:167:ASP:O	1:F:168:LYS:HB2	2.11	0.50
1:B:319:LEU:CD2	1:B:319:LEU:H	2.24	0.50
1:E:575:ASP:OD1	1:E:575:ASP:C	2.55	0.50
1:F:134:HIS:HB3	1:F:136:ILE:HD12	1.94	0.50
1:F:601:ASN:HD21	1:F:603:PRO:HD2	1.69	0.50
1:B:215:GLU:O	1:B:216:ASN:C	2.55	0.50
1:B:331:TYR:CZ	1:B:375:THR:HG23	2.46	0.50
1:D:83:HIS:HA	1:D:314:ARG:NH1	2.26	0.50
1:B:685:ASN:HD21	1:B:687:ASN:H	1.57	0.49
1:B:179:ASN:OD1	1:B:207:PRO:HA	2.12	0.49
1:A:456:LYS:HA	1:A:456:LYS:CE	2.42	0.49
1:A:570:VAL:O	1:A:570:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:LYS:HD3	1:B:168:LYS:N	2.26	0.49
1:D:186:THR:O	1:D:187:ARG:C	2.53	0.49
1:B:490:LEU:CD1	1:B:494:ARG:HE	2.25	0.49
1:E:293:GLY:HA3	1:E:677:LYS:HB2	1.94	0.49
1:A:599:HIS:HE1	1:A:632:TYR:OH	1.96	0.49
1:B:40:THR:O	1:B:639:TYR:HB2	2.13	0.49
1:D:61:GLY:O	1:D:77:ARG:HD3	2.12	0.49
1:D:685:ASN:HD22	1:D:687:ASN:H	1.60	0.49
1:E:408:MET:HE1	1:E:480:GLU:HG2	1.93	0.49
1:E:547:PRO:HB2	1:E:613:TYR:CD2	2.48	0.49
1:F:172:ILE:CD1	1:F:233:ALA:HB2	2.40	0.49
1:F:547:PRO:HG2	1:F:613:TYR:CE2	2.47	0.49
1:F:746:GLU:HG2	5:F:2193:HOH:O	2.12	0.49
1:B:431:HIS:CD2	1:B:434:VAL:N	2.77	0.49
1:B:496:MET:HE3	1:B:496:MET:CA	2.41	0.49
1:C:30:MET:HE2	1:C:639:TYR:CZ	2.48	0.49
1:D:318:GLU:O	1:D:319:LEU:CD2	2.58	0.49
1:D:547:PRO:O	1:D:551:ILE:HG13	2.13	0.49
1:A:331:TYR:CZ	1:A:375:THR:HG23	2.47	0.49
1:B:293:GLY:HA3	1:B:677:LYS:HB2	1.93	0.49
1:C:320:ASP:C	1:C:320:ASP:OD1	2.56	0.49
1:F:99:PRO:HG3	1:F:151:PHE:CD2	2.48	0.49
1:B:352:CYS:C	1:B:355:PRO:HD2	2.38	0.49
1:B:452:PRO:HB2	1:B:455:VAL:CG2	2.29	0.49
1:E:439:ARG:NH2	1:E:471:ASP:OD1	2.44	0.49
1:B:449:GLY:CA	1:B:497:ASN:ND2	2.76	0.48
1:F:199:TYR:O	1:F:251:SER:HA	2.12	0.48
1:B:97:ILE:HD11	1:B:161:VAL:CG1	2.41	0.48
1:B:602:GLN:N	1:B:603:PRO:HD3	2.28	0.48
1:F:593:ASN:ND2	5:F:2147:HOH:O	2.45	0.48
1:B:99:PRO:HG3	1:B:151:PHE:CD2	2.47	0.48
1:B:269:ASP:HB2	1:B:274:LEU:HG	1.95	0.48
1:B:407:TYR:CZ	1:B:412:LYS:HE2	2.47	0.48
1:B:415:ASP:CG	1:B:418:THR:OG1	2.56	0.48
1:D:408:MET:HE1	1:D:480:GLU:HG2	1.96	0.48
1:E:601:ASN:C	1:E:601:ASN:HD22	2.21	0.48
1:B:496:MET:CE	1:B:499:LYS:HD2	2.43	0.48
1:C:86:SER:HB2	1:C:87:PRO:HD2	1.96	0.48
1:D:394:MET:CE	1:D:532:THR:HG21	2.43	0.48
1:E:365:ASN:O	1:E:369:GLN:HG2	2.13	0.48
1:C:700:ASN:ND2	1:C:735:ASN:HB3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:ILE:HD13	1:D:326:ILE:CD1	2.42	0.48
1:A:431:HIS:HB3	1:A:434:VAL:O	2.13	0.48
1:B:547:PRO:HG2	1:B:613:TYR:CD2	2.44	0.48
1:C:47:ILE:HD13	1:C:47:ILE:N	2.29	0.48
1:D:314:ARG:NE	1:D:343:ASP:OD2	2.39	0.48
1:E:407:TYR:HD1	1:E:408:MET:HE1	1.65	0.48
1:F:354:PHE:N	1:F:355:PRO:CD	2.77	0.48
1:B:559:MET:HG2	5:B:2125:HOH:O	2.12	0.48
1:D:49:ARG:O	1:D:50:PRO:C	2.56	0.48
1:B:547:PRO:CB	1:B:613:TYR:CD2	2.97	0.48
1:B:622:TYR:C	1:B:622:TYR:CD2	2.92	0.48
1:A:77:ARG:HH21	1:A:109:GLU:HA	1.77	0.48
1:D:347:TRP:CD2	1:D:394:MET:HE2	2.48	0.48
1:B:56:TRP:CE2	1:B:147:VAL:HG11	2.49	0.47
1:B:483:ARG:HE	1:B:483:ARG:HB3	1.24	0.47
1:B:744:LYS:O	1:B:747:ASP:HB2	2.13	0.47
1:D:555:GLY:C	1:D:559:MET:HE2	2.39	0.47
1:D:558:GLU:CD	1:D:558:GLU:H	2.23	0.47
1:F:559:MET:HE2	1:F:563:MET:HG2	1.96	0.47
1:D:496:MET:HE2	1:D:499:LYS:HZ2	1.79	0.47
1:E:331:TYR:CZ	1:E:375:THR:HG23	2.49	0.47
1:A:416:ILE:HD11	1:A:481:LEU:CG	2.43	0.47
1:B:377:LEU:CD2	1:B:418:THR:HG21	2.45	0.47
1:F:22:TRP:NE1	5:F:2002:HOH:O	2.19	0.47
1:F:700:ASN:ND2	1:F:735:ASN:HB3	2.30	0.47
1:A:361:TYR:N	1:A:362:PRO:CD	2.77	0.47
1:A:408:MET:HE1	1:A:480:GLU:HG2	1.96	0.47
1:B:90:ASN:OD1	1:B:91:ASP:N	2.47	0.47
1:B:209:THR:O	1:B:209:THR:CG2	2.62	0.47
1:D:210:TYR:CD1	1:D:210:TYR:C	2.93	0.47
1:E:38:LEU:HD12	1:E:588:GLU:HG3	1.97	0.47
1:E:546:ASP:N	1:E:547:PRO:HD3	2.30	0.47
1:F:210:TYR:CD1	1:F:210:TYR:C	2.93	0.47
1:B:95:PHE:HB2	1:B:164:ASP:O	2.14	0.47
1:C:677:LYS:HE2	5:C:2109:HOH:O	2.14	0.47
1:F:319:LEU:N	1:F:319:LEU:CD2	2.77	0.47
1:A:685:ASN:ND2	1:A:685:ASN:C	2.73	0.47
1:C:107:ASP:HB3	1:C:110:LYS:HB2	1.96	0.47
1:C:685:ASN:ND2	1:C:685:ASN:C	2.73	0.47
1:B:477:LEU:HD12	1:B:481:LEU:HD11	1.97	0.47
1:C:564:MET:HE3	1:C:607:MET:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:TRP:CE3	1:B:534:GLY:HA2	2.50	0.46
1:D:559:MET:HB3	5:D:2112:HOH:O	2.15	0.46
1:D:700:ASN:HD22	1:D:735:ASN:HB3	1.80	0.46
1:F:172:ILE:HD13	1:F:233:ALA:CB	2.41	0.46
1:A:455:VAL:O	1:A:456:LYS:HB2	2.15	0.46
1:B:361:TYR:N	1:B:362:PRO:CD	2.78	0.46
1:D:392:GLY:HA2	1:D:436:SER:OG	2.15	0.46
1:F:416:ILE:O	1:F:417:LYS:C	2.58	0.46
1:D:182:ILE:HG22	1:D:201:ILE:HG12	1.97	0.46
1:D:533:GLU:OE2	1:D:585:GLU:OE2	2.33	0.46
1:B:314:ARG:HG3	1:B:315:LYS:O	2.16	0.46
1:C:504:LYS:HG3	1:C:504:LYS:H	1.58	0.46
1:C:520:SER:HA	1:C:521:PRO:C	2.41	0.46
1:D:312:PHE:HA	1:D:313:PRO:C	2.41	0.46
1:D:602:GLN:N	1:D:603:PRO:CD	2.79	0.46
1:D:738:ASN:ND2	1:D:741:ARG:HB2	2.31	0.46
1:A:609:TYR:CZ	1:A:660:TYR:HB2	2.51	0.46
1:C:744:LYS:CE	1:C:747:ASP:OD2	2.61	0.46
1:F:40:THR:HG21	1:F:637:ASP:HB2	1.97	0.46
1:F:601:ASN:HD22	1:F:603:PRO:HD2	1.72	0.46
1:A:709:ASN:HD21	1:A:728:THR:H	1.63	0.46
1:D:555:GLY:CA	1:D:559:MET:CE	2.85	0.46
1:F:544:PHE:CE2	1:F:606:HIS:CE1	3.04	0.46
1:F:611:TYR:HB2	1:F:620:ALA:HB2	1.98	0.46
1:B:477:LEU:CD1	1:B:481:LEU:CD1	2.94	0.46
1:C:167:ASP:O	1:C:168:LYS:HB2	2.15	0.46
1:D:350:PHE:C	1:D:350:PHE:CD2	2.93	0.46
1:A:107:ASP:HB3	1:A:110:LYS:HB2	1.97	0.46
1:A:186:THR:O	1:A:187:ARG:C	2.58	0.46
1:B:186:THR:O	1:B:187:ARG:C	2.58	0.46
1:D:237:PHE:CD2	1:D:237:PHE:N	2.84	0.46
1:E:496:MET:HB3	1:E:499:LYS:HE3	1.99	0.45
1:F:142:PRO:HA	1:F:147:VAL:HA	1.98	0.45
1:B:546:ASP:N	1:B:547:PRO:HD3	2.31	0.45
1:F:502:PHE:CG	1:F:553:LEU:HD13	2.52	0.45
1:A:101:VAL:HG13	1:A:136:ILE:HD11	1.97	0.45
1:E:483:ARG:HB3	1:E:484:PRO:CD	2.46	0.45
1:E:524:PRO:O	1:E:535:ASN:HB2	2.17	0.45
1:F:504:LYS:HB2	1:F:504:LYS:HE3	1.69	0.45
1:B:441:GLY:C	1:B:443:GLU:OE1	2.59	0.45
1:B:609:TYR:CZ	1:B:660:TYR:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:PHE:CD2	1:C:350:PHE:C	2.94	0.45
1:E:26:VAL:HG11	1:E:124:PRO:HG3	1.99	0.45
1:F:570:VAL:O	1:F:571:PRO:C	2.59	0.45
1:A:350:PHE:CD2	1:A:350:PHE:C	2.94	0.45
1:B:376:TYR:CD1	1:B:380:GLY:C	2.95	0.45
1:D:258:GLN:HG3	1:D:258:GLN:O	2.17	0.45
1:F:601:ASN:ND2	1:F:603:PRO:CD	2.64	0.45
1:D:99:PRO:HG3	1:D:151:PHE:CD2	2.52	0.45
1:D:214:VAL:HA	1:D:218:ASN:O	2.17	0.45
1:D:347:TRP:CZ3	1:D:394:MET:HE2	2.52	0.45
1:D:659:PHE:HE2	1:D:691:ILE:HD11	1.82	0.45
1:B:92:TYR:CD2	1:B:92:TYR:C	2.95	0.45
1:C:90:ASN:HB3	1:C:189:SER:OG	2.16	0.45
1:D:220:GLN:HB3	1:D:223:VAL:CG2	2.46	0.45
1:A:216:ASN:N	1:A:216:ASN:HD22	2.14	0.45
1:C:459:GLU:HG2	1:C:531:PHE:O	2.17	0.45
1:D:612:ASP:OD2	1:D:671:MET:O	2.34	0.45
1:A:575:ASP:OD1	1:A:575:ASP:C	2.60	0.45
1:D:290:GLU:O	1:D:679:ALA:HA	2.16	0.45
1:D:566:SER:O	1:D:570:VAL:HG13	2.17	0.45
1:E:345:GLY:HA3	1:E:385:TRP:CE2	2.51	0.45
1:A:510:ARG:HG3	1:A:522:PHE:CD1	2.52	0.45
1:B:454:ASP:OD2	1:B:514:GLU:N	2.45	0.44
1:B:564:MET:HE2	1:B:611:TYR:CE1	2.50	0.44
1:F:407:TYR:HD1	1:F:408:MET:CE	2.23	0.44
1:F:532:THR:HG22	1:F:533:GLU:HG2	1.99	0.44
1:A:347:TRP:CE3	1:A:394:MET:HE2	2.52	0.44
1:B:597:TYR:OH	1:B:599:HIS:HD2	1.99	0.44
1:D:446:ASN:HD22	1:D:446:ASN:HA	1.63	0.44
1:E:461:ALA:O	1:E:465:LEU:HG	2.17	0.44
1:F:477:LEU:HG	1:F:481:LEU:HD22	1.99	0.44
1:B:317:TYR:CD1	1:B:317:TYR:C	2.94	0.44
1:B:456:LYS:HD2	1:B:456:LYS:HA	1.79	0.44
1:D:26:VAL:HG11	1:D:124:PRO:HG3	1.99	0.44
1:E:415:ASP:OD2	1:E:418:THR:OG1	2.34	0.44
1:E:431:HIS:HD2	1:E:434:VAL:H	1.64	0.44
1:F:416:ILE:HG23	1:F:417:LYS:N	2.31	0.44
1:A:394:MET:HE3	1:A:532:THR:HG21	2.00	0.44
1:B:269:ASP:OD2	1:B:277:LYS:NZ	2.40	0.44
1:F:520:SER:HA	1:F:521:PRO:C	2.42	0.44
1:A:56:TRP:CZ2	1:A:81:GLN:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:ASP:HB2	1:C:274:LEU:HG	1.98	0.44
1:E:353:LEU:HD13	1:E:353:LEU:C	2.43	0.44
1:F:575:ASP:OD1	1:F:575:ASP:C	2.60	0.44
1:A:26:VAL:HG11	1:A:124:PRO:HG3	1.99	0.44
1:A:681:LEU:O	1:A:688:SER:HA	2.17	0.44
1:B:510:ARG:HG3	1:B:522:PHE:CD1	2.52	0.44
1:B:529:ASP:HB3	1:B:530:ALA:H	1.59	0.44
1:D:329:SER:C	1:D:331:TYR:H	2.26	0.44
1:E:56:TRP:CE2	1:E:147:VAL:HG11	2.53	0.44
1:E:354:PHE:N	1:E:355:PRO:CD	2.80	0.44
1:F:281:ALA:O	1:F:284:GLN:HB3	2.17	0.44
1:A:456:LYS:N	1:A:456:LYS:HD2	2.32	0.44
1:B:52:GLY:O	1:B:314:ARG:HB2	2.17	0.44
1:B:559:MET:HG2	1:B:559:MET:H	1.62	0.44
1:D:707:SER:OG	1:D:730:LYS:HB3	2.18	0.44
1:E:607:MET:HE2	1:E:607:MET:HB3	1.83	0.44
1:F:524:PRO:O	1:F:535:ASN:HB2	2.17	0.44
1:A:75:LYS:HE2	1:A:114:TRP:CD1	2.53	0.44
1:A:416:ILE:O	1:A:416:ILE:HG12	2.18	0.44
1:A:419:LEU:C	1:A:419:LEU:HD12	2.42	0.44
1:A:431:HIS:HD2	1:A:433:GLU:N	2.12	0.44
1:E:481:LEU:HD12	1:E:481:LEU:HA	1.87	0.44
1:F:375:THR:HG21	1:F:383:PRO:CD	2.40	0.44
1:F:528:GLY:O	1:F:529:ASP:HB3	2.18	0.44
1:F:756:LEU:HD12	1:F:756:LEU:HA	1.67	0.44
1:C:616:GLN:HA	1:C:618:TRP:CZ3	2.53	0.43
1:D:209:THR:HB	1:D:237:PHE:HA	2.00	0.43
1:D:353:LEU:C	1:D:353:LEU:HD13	2.43	0.43
1:D:551:ILE:HG12	1:D:560:PHE:CD2	2.53	0.43
1:D:94:GLN:NE2	1:D:187:ARG:HG2	2.33	0.43
1:C:58:PRO:HG3	1:C:127:TYR:CE1	2.52	0.43
1:D:188:ASN:ND2	1:D:190:GLY:H	2.00	0.43
1:D:394:MET:HE1	1:D:532:THR:HG22	1.99	0.43
1:F:352:CYS:C	1:F:355:PRO:HD2	2.44	0.43
1:F:420:TYR:O	1:F:421:GLU:C	2.61	0.43
1:F:601:ASN:HD22	1:F:601:ASN:C	2.26	0.43
1:D:469:TYR:HA	1:D:545:HIS:CE1	2.53	0.43
1:E:547:PRO:HG2	1:E:613:TYR:CE2	2.53	0.43
1:F:110:LYS:HD2	1:F:110:LYS:HA	1.51	0.43
1:F:175:ILE:O	1:F:175:ILE:HG22	2.18	0.43
1:B:320:ASP:OD1	1:B:320:ASP:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:320:ASP:C	1:F:320:ASP:OD1	2.61	0.43
1:F:347:TRP:CE3	1:F:394:MET:HE2	2.52	0.43
1:A:32:SER:HB3	5:A:2008:HOH:O	2.18	0.43
1:B:564:MET:HE2	1:B:564:MET:HB3	1.69	0.43
1:C:713:HIS:CE1	1:C:718:LEU:HD23	2.54	0.43
1:D:306:LEU:O	1:D:310:LEU:HG	2.19	0.43
1:E:419:LEU:C	1:E:419:LEU:CD1	2.92	0.43
1:F:455:VAL:O	1:F:456:LYS:HB2	2.19	0.43
1:F:625:ARG:NH1	1:F:701:PHE:HB3	2.34	0.43
1:A:681:LEU:N	1:A:681:LEU:HD23	2.33	0.43
1:B:350:PHE:CD2	1:B:350:PHE:C	2.96	0.43
1:B:523:SER:HA	1:B:524:PRO:HD3	1.86	0.43
1:D:494:ARG:O	1:D:497:ASN:HB2	2.19	0.43
1:B:107:ASP:HB3	1:B:110:LYS:HB2	2.00	0.43
1:B:483:ARG:NE	1:B:484:PRO:HD2	2.34	0.43
1:B:490:LEU:HD21	1:B:494:ARG:NH2	2.33	0.43
1:C:40:THR:HG21	1:C:637:ASP:HB2	2.01	0.43
1:E:504:LYS:H	1:E:504:LYS:HG3	1.64	0.43
1:F:92:TYR:CD2	1:F:92:TYR:C	2.97	0.43
1:A:550:LEU:HD11	1:A:554:MET:HE3	2.01	0.43
1:F:168:LYS:HD3	1:F:168:LYS:HA	1.59	0.43
1:F:738:ASN:OD1	1:F:738:ASN:C	2.61	0.43
1:B:527:TRP:CE2	1:B:586:ILE:HG12	2.53	0.43
1:D:92:TYR:CD2	1:D:92:TYR:C	2.97	0.43
1:D:700:ASN:ND2	1:D:735:ASN:HB3	2.34	0.43
1:E:77:ARG:HH21	1:E:109:GLU:HA	1.83	0.43
1:E:167:ASP:O	1:E:168:LYS:HB2	2.19	0.43
1:A:685:ASN:HD22	1:A:687:ASN:H	1.63	0.42
1:B:220:GLN:HE21	1:B:223:VAL:HG21	1.83	0.42
1:B:453:TYR:O	1:B:453:TYR:CD1	2.71	0.42
1:B:607:MET:HE2	1:B:607:MET:HB3	1.86	0.42
1:E:598:ALA:O	1:E:601:ASN:HB3	2.18	0.42
1:A:345:GLY:HA3	1:A:385:TRP:CE2	2.54	0.42
1:B:270:ASN:OD1	1:B:270:ASN:C	2.61	0.42
1:C:56:TRP:CE2	1:C:147:VAL:HG11	2.54	0.42
1:D:570:VAL:HA	1:D:571:PRO:HD3	1.80	0.42
1:E:101:VAL:HG13	1:E:136:ILE:HD11	2.01	0.42
1:F:312:PHE:HA	1:F:313:PRO:C	2.43	0.42
1:F:417:LYS:O	1:F:421:GLU:HG3	2.19	0.42
1:A:100:ILE:HG12	1:A:160:TYR:HB2	2.01	0.42
1:A:616:GLN:HA	1:A:618:TRP:CZ3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:PHE:HE1	1:B:507:LYS:O	2.02	0.42
1:B:719:ARG:O	1:B:720:HIS:C	2.61	0.42
1:C:188:ASN:ND2	1:C:190:GLY:H	2.06	0.42
1:D:423:LEU:O	1:D:427:THR:HG23	2.19	0.42
1:D:466:GLU:O	1:D:470:ASP:CG	2.62	0.42
1:A:319:LEU:HD22	1:A:319:LEU:N	2.35	0.42
1:C:515:ASP:OD1	1:C:515:ASP:C	2.63	0.42
1:D:709:ASN:HD21	1:D:728:THR:N	2.17	0.42
1:B:38:LEU:HD12	1:B:588:GLU:HG3	2.01	0.42
1:B:689:LEU:HD12	1:B:727:GLY:O	2.19	0.42
1:C:709:ASN:HD21	1:C:727:GLY:HA3	1.85	0.42
1:D:496:MET:HE3	1:D:496:MET:HB3	1.84	0.42
1:E:573:ILE:HG12	1:E:574:PHE:H	1.84	0.42
1:B:477:LEU:HG	1:B:481:LEU:HD13	2.02	0.42
1:B:555:GLY:HA3	1:B:559:MET:HE2	2.02	0.42
1:C:541:TRP:CG	1:C:607:MET:HG3	2.55	0.42
1:D:184:TYR:CE1	1:D:197:LYS:HE3	2.55	0.42
1:E:709:ASN:HD21	1:E:728:THR:H	1.67	0.42
1:B:496:MET:CE	1:B:496:MET:HA	2.47	0.42
1:D:709:ASN:HD21	1:D:727:GLY:HA3	1.85	0.42
1:F:739:LEU:HD12	1:F:739:LEU:HA	1.65	0.42
1:A:564:MET:CE	1:A:607:MET:HE3	2.49	0.42
1:B:441:GLY:HA2	1:B:443:GLU:OE1	2.19	0.42
1:B:520:SER:HA	1:B:521:PRO:C	2.45	0.42
1:A:419:LEU:HD12	1:A:419:LEU:O	2.19	0.42
1:B:209:THR:O	1:B:209:THR:HG23	2.20	0.42
1:B:353:LEU:C	1:B:353:LEU:HD13	2.44	0.42
1:B:444:TYR:HH	1:B:455:VAL:HG12	1.81	0.42
1:D:34:SER:HB3	1:D:42:ASN:OD1	2.20	0.42
1:D:443:GLU:CD	1:D:443:GLU:H	2.26	0.42
1:F:607:MET:HE2	1:F:607:MET:HB3	1.94	0.42
1:A:407:TYR:CE1	1:A:408:MET:HE1	2.55	0.42
1:C:319:LEU:HD12	1:C:319:LEU:HA	1.86	0.42
1:D:616:GLN:HA	1:D:618:TRP:CZ3	2.54	0.42
1:F:633:THR:HB	1:F:634:PRO:HD2	2.02	0.42
1:B:496:MET:CE	1:B:499:LYS:CD	2.98	0.41
1:B:599:HIS:HE1	1:B:632:TYR:OH	2.03	0.41
1:D:173:LYS:HA	1:D:224:ALA:O	2.20	0.41
1:B:51:TRP:CH2	1:B:364:VAL:HG21	2.55	0.41
1:B:431:HIS:HA	1:B:432:PRO:HD3	1.83	0.41
1:B:689:LEU:CD2	1:B:723:LEU:HD22	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:730:LYS:HE2	1:C:732:ASP:OD1	2.20	0.41
1:D:266:LEU:HD22	1:D:274:LEU:HD11	2.02	0.41
1:D:663:CYS:O	1:D:664:PRO:C	2.61	0.41
1:F:209:THR:O	1:F:209:THR:HG23	2.20	0.41
1:F:225:GLU:C	1:F:226:GLN:HG2	2.45	0.41
1:F:135:ASP:HB3	1:F:154:PRO:HG3	2.01	0.41
1:A:167:ASP:HA	1:A:229:ASP:O	2.21	0.41
1:A:570:VAL:HA	1:A:571:PRO:HD3	1.90	0.41
1:C:572:PRO:HB2	1:C:589:MET:HE3	2.01	0.41
1:D:319:LEU:HD22	1:D:319:LEU:HA	1.73	0.41
1:D:354:PHE:N	1:D:355:PRO:CD	2.84	0.41
1:D:533:GLU:O	1:D:601:ASN:ND2	2.53	0.41
1:E:523:SER:HA	1:E:524:PRO:HD2	1.78	0.41
1:E:551:ILE:HG12	1:E:560:PHE:CG	2.56	0.41
1:A:99:PRO:HG3	1:A:151:PHE:CD2	2.55	0.41
1:A:123:THR:HB	1:A:124:PRO:HD2	2.00	0.41
1:A:744:LYS:NZ	1:A:747:ASP:OD2	2.46	0.41
1:B:193:PRO:HG2	1:B:328:TYR:OH	2.21	0.41
1:B:373:ILE:HD13	1:B:373:ILE:HA	1.76	0.41
1:B:601:ASN:C	1:B:603:PRO:CD	2.93	0.41
1:D:185:THR:CG2	1:D:198:ASN:HB3	2.51	0.41
1:C:165:ALA:O	1:C:166:PHE:HB2	2.20	0.41
1:C:444:TYR:HB3	1:C:452:PRO:HD3	2.02	0.41
1:E:206:LYS:HA	1:E:207:PRO:HD3	1.92	0.41
1:E:744:LYS:O	1:E:745:GLU:C	2.64	0.41
1:F:609:TYR:CZ	1:F:660:TYR:HB2	2.56	0.41
1:B:60:THR:O	1:B:77:ARG:NH1	2.54	0.41
1:B:80:LYS:HE3	1:B:94:GLN:HB2	2.01	0.41
1:B:483:ARG:CZ	1:B:484:PRO:HD2	2.51	0.41
1:B:623:TRP:O	1:B:627:VAL:HG23	2.21	0.41
1:D:428:GLU:HA	1:D:442:TYR:CD2	2.56	0.41
1:E:165:ALA:O	1:E:166:PHE:HB2	2.20	0.41
1:E:210:TYR:CD1	1:E:210:TYR:C	2.99	0.41
1:E:350:PHE:CD2	1:E:350:PHE:C	2.97	0.41
1:F:496:MET:HE3	1:F:499:LYS:HE3	1.86	0.41
1:F:756:LEU:O	1:F:757:GLU:CB	2.69	0.41
1:C:167:ASP:HA	1:C:229:ASP:O	2.20	0.41
1:A:240:ARG:HG3	1:A:243:GLU:HB2	2.03	0.41
1:B:360:MET:SD	1:B:681:LEU:HD22	2.60	0.41
1:B:430:VAL:CG2	1:B:440:LEU:HA	2.50	0.41
1:B:709:ASN:HD21	1:B:728:THR:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:LEU:HD12	1:D:219:LEU:HA	1.93	0.41
1:E:408:MET:HE2	1:E:408:MET:N	2.36	0.41
1:F:212:ALA:HB2	1:F:221:GLU:HA	2.03	0.41
1:F:408:MET:HB2	5:F:2121:HOH:O	2.21	0.41
1:B:153:PHE:CD1	1:B:159:SER:HB3	2.56	0.41
1:C:633:THR:HB	1:C:634:PRO:HD2	2.02	0.41
1:D:240:ARG:NE	5:D:2063:HOH:O	2.54	0.41
1:D:394:MET:CE	1:D:532:THR:CG2	2.99	0.41
1:D:564:MET:CE	1:D:607:MET:HE3	2.50	0.41
1:A:216:ASN:HD22	1:A:216:ASN:H	1.67	0.40
1:B:394:MET:HE1	1:B:533:GLU:HG3	2.02	0.40
1:C:546:ASP:N	1:C:547:PRO:HD3	2.35	0.40
1:F:360:MET:HB2	1:F:361:TYR:CE2	2.56	0.40
1:B:553:LEU:HD23	1:B:553:LEU:HA	1.82	0.40
1:C:374:ASN:HD22	1:C:374:ASN:HA	1.69	0.40
1:D:667:ASP:OD1	1:D:667:ASP:C	2.65	0.40
1:E:550:LEU:HD11	1:E:554:MET:HE2	1.95	0.40
1:B:99:PRO:HB2	1:B:136:ILE:HD13	2.03	0.40
1:B:490:LEU:HD11	1:B:494:ARG:HE	1.85	0.40
1:C:607:MET:HE2	1:C:607:MET:HB3	1.93	0.40
1:D:446:ASN:ND2	1:D:494:ARG:CZ	2.84	0.40
1:D:553:LEU:HD23	1:D:553:LEU:HA	1.81	0.40
1:E:601:ASN:HD22	1:E:604:ILE:H	1.69	0.40
1:F:69:TYR:CD2	1:F:69:TYR:C	2.99	0.40
1:F:140:MET:HA	1:F:148:LEU:O	2.21	0.40
1:F:387:SER:HA	1:F:388:PRO:HA	1.82	0.40
1:A:53:MET:HB3	1:A:145:ARG:HG2	2.04	0.40
1:B:442:TYR:O	1:B:443:GLU:C	2.64	0.40
1:C:168:LYS:HD3	1:C:168:LYS:HA	1.83	0.40
1:E:179:ASN:OD1	1:E:207:PRO:HA	2.22	0.40
1:E:315:LYS:HE2	1:E:317:TYR:OH	2.21	0.40
1:F:329:SER:C	1:F:331:TYR:H	2.27	0.40
1:A:320:ASP:C	1:A:320:ASP:OD1	2.64	0.40
1:D:564:MET:HE2	1:D:611:TYR:CE2	2.55	0.40
1:D:748:MET:HA	1:D:749:PRO:HD3	1.94	0.40
1:F:506:SER:O	1:F:507:LYS:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	734/744 (99%)	710 (97%)	23 (3%)	1 (0%)	48	50
1	B	734/744 (99%)	693 (94%)	41 (6%)	0	100	100
1	C	734/744 (99%)	711 (97%)	23 (3%)	0	100	100
1	D	736/744 (99%)	700 (95%)	35 (5%)	1 (0%)	48	50
1	E	735/744 (99%)	705 (96%)	30 (4%)	0	100	100
1	F	736/744 (99%)	701 (95%)	35 (5%)	0	100	100
All	All	4409/4464 (99%)	4220 (96%)	187 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	529	ASP
1	A	529	ASP

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	632/643 (98%)	610 (96%)	22 (4%)	32	35
1	B	627/643 (98%)	598 (95%)	29 (5%)	24	25
1	C	630/643 (98%)	613 (97%)	17 (3%)	39	45
1	D	627/643 (98%)	611 (97%)	16 (3%)	40	46
1	E	629/643 (98%)	605 (96%)	24 (4%)	29	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	628/643 (98%)	603 (96%)	25 (4%)	28	29
All	All	3773/3858 (98%)	3640 (96%)	133 (4%)	32	35

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	ILE
1	A	209	THR
1	A	215	GLU
1	A	237	PHE
1	A	238	LYS
1	A	385	TRP
1	A	408	MET
1	A	416	ILE
1	A	419	LEU
1	A	456	LYS
1	A	460	ASN
1	A	481	LEU
1	A	496	MET
1	A	519	GLN
1	A	539	TYR
1	A	573	ILE
1	A	593	ASN
1	A	601	ASN
1	A	685	ASN
1	A	692	ASP
1	A	739	LEU
1	A	746	GLU
1	B	34	SER
1	B	185	THR
1	B	188	ASN
1	B	209	THR
1	B	237	PHE
1	B	238	LYS
1	B	307	TYR
1	B	385	TRP
1	B	399	SER
1	B	425	HIS
1	B	430	VAL
1	B	433	GLU
1	B	440	LEU
1	B	443	GLU

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Mol	Chain	Res	Type
1	B	455	VAL
1	B	456	LYS
1	B	459	GLU
1	B	460	ASN
1	B	482	LYS
1	B	520	SER
1	B	539	TYR
1	B	559	MET
1	B	564	MET
1	B	607	MET
1	B	685	ASN
1	B	730	LYS
1	B	736	ARG
1	B	739	LEU
1	B	746	GLU
1	C	105	VAL
1	C	172	ILE
1	C	209	THR
1	C	237	PHE
1	C	319	LEU
1	C	385	TRP
1	C	443	GLU
1	C	460	ASN
1	C	481	LEU
1	C	493	LYS
1	C	504	LYS
1	C	539	TYR
1	C	573	ILE
1	C	593	ASN
1	C	685	ASN
1	C	712	ASP
1	C	739	LEU
1	D	34	SER
1	D	185	THR
1	D	194	GLU
1	D	209	THR
1	D	215	GLU
1	D	237	PHE
1	D	319	LEU
1	D	443	GLU
1	D	455	VAL
1	D	456	LYS

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Mol	Chain	Res	Type
1	D	539	TYR
1	D	566	SER
1	D	685	ASN
1	D	705	SER
1	D	739	LEU
1	D	746	GLU
1	E	77	ARG
1	E	110	LYS
1	E	209	THR
1	E	237	PHE
1	E	240	ARG
1	E	385	TRP
1	E	416	ILE
1	E	419	LEU
1	E	433	GLU
1	E	443	GLU
1	E	456	LYS
1	E	460	ASN
1	E	481	LEU
1	E	482	LYS
1	E	504	LYS
1	E	519	GLN
1	E	539	TYR
1	E	573	ILE
1	E	601	ASN
1	E	685	ASN
1	E	692	ASP
1	E	712	ASP
1	E	731	VAL
1	E	739	LEU
1	F	34	SER
1	F	77	ARG
1	F	110	LYS
1	F	168	LYS
1	F	209	THR
1	F	215	GLU
1	F	237	PHE
1	F	268	LYS
1	F	319	LEU
1	F	350	PHE
1	F	385	TRP
1	F	416	ILE

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Mol	Chain	Res	Type
1	F	419	LEU
1	F	460	ASN
1	F	482	LYS
1	F	504	LYS
1	F	519	GLN
1	F	539	TYR
1	F	573	ILE
1	F	577	SER
1	F	601	ASN
1	F	685	ASN
1	F	706	MET
1	F	739	LEU
1	F	756	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (137) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	81	GLN
1	A	84	GLN
1	A	94	GLN
1	A	188	ASN
1	A	216	ASN
1	A	220	GLN
1	A	226	GLN
1	A	264	ASN
1	A	283	ASN
1	A	358	ASN
1	A	374	ASN
1	A	431	HIS
1	A	446	ASN
1	A	593	ASN
1	A	599	HIS
1	A	601	ASN
1	A	685	ASN
1	A	700	ASN
1	A	709	ASN
1	B	59	GLN
1	B	84	GLN
1	B	188	ASN
1	B	216	ASN
1	B	220	GLN

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Mol	Chain	Res	Type
1	B	226	GLN
1	B	246	ASN
1	B	264	ASN
1	B	283	ASN
1	B	324	GLN
1	B	358	ASN
1	B	374	ASN
1	B	398	ASN
1	B	425	HIS
1	B	431	HIS
1	B	446	ASN
1	B	497	ASN
1	B	513	ASN
1	B	519	GLN
1	B	593	ASN
1	B	599	HIS
1	B	685	ASN
1	B	700	ASN
1	B	709	ASN
1	B	713	HIS
1	B	716	ASN
1	C	59	GLN
1	C	84	GLN
1	C	188	ASN
1	C	216	ASN
1	C	220	GLN
1	C	244	GLN
1	C	246	ASN
1	C	258	GLN
1	C	264	ASN
1	C	283	ASN
1	C	358	ASN
1	C	374	ASN
1	C	425	HIS
1	C	593	ASN
1	C	599	HIS
1	C	685	ASN
1	C	700	ASN
1	C	709	ASN
1	C	713	HIS
1	D	59	GLN
1	D	74	ASN

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Mol	Chain	Res	Type
1	D	81	GLN
1	D	84	GLN
1	D	158	HIS
1	D	188	ASN
1	D	216	ASN
1	D	226	GLN
1	D	246	ASN
1	D	264	ASN
1	D	283	ASN
1	D	324	GLN
1	D	358	ASN
1	D	369	GLN
1	D	374	ASN
1	D	398	ASN
1	D	431	HIS
1	D	446	ASN
1	D	519	GLN
1	D	593	ASN
1	D	599	HIS
1	D	685	ASN
1	D	700	ASN
1	D	709	ASN
1	D	713	HIS
1	D	716	ASN
1	E	59	GLN
1	E	84	GLN
1	E	94	GLN
1	E	188	ASN
1	E	220	GLN
1	E	226	GLN
1	E	264	ASN
1	E	283	ASN
1	E	358	ASN
1	E	369	GLN
1	E	374	ASN
1	E	398	ASN
1	E	431	HIS
1	E	446	ASN
1	E	519	GLN
1	E	593	ASN
1	E	599	HIS
1	E	601	ASN

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Mol	Chain	Res	Type
1	E	685	ASN
1	E	700	ASN
1	E	709	ASN
1	E	713	HIS
1	F	84	GLN
1	F	103	GLN
1	F	158	HIS
1	F	188	ASN
1	F	244	GLN
1	F	264	ASN
1	F	283	ASN
1	F	334	GLN
1	F	358	ASN
1	F	374	ASN
1	F	425	HIS
1	F	429	ASN
1	F	431	HIS
1	F	446	ASN
1	F	519	GLN
1	F	593	ASN
1	F	599	HIS
1	F	601	ASN
1	F	616	GLN
1	F	626	GLN
1	F	685	ASN
1	F	700	ASN
1	F	709	ASN
1	F	716	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

12 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	Z5L	G	1	2	12,13,13	0.86	1 (8%)	14,18,18	0.73	0
2	MAN	G	2	3,2	11,11,12	0.44	0	15,15,17	1.18	1 (6%)
2	Z5L	H	1	2	12,13,13	0.78	1 (8%)	14,18,18	0.80	0
2	MAN	H	2	3,2	11,11,12	0.60	0	15,15,17	1.43	2 (13%)
2	Z5L	I	1	2	12,13,13	0.80	1 (8%)	14,18,18	1.06	1 (7%)
2	MAN	I	2	3,2	11,11,12	0.59	0	15,15,17	1.45	2 (13%)
2	Z5L	J	1	2	12,13,13	0.92	1 (8%)	14,18,18	0.62	0
2	MAN	J	2	3,2	11,11,12	0.38	0	15,15,17	1.19	1 (6%)
2	Z5L	K	1	2	12,13,13	0.68	0	14,18,18	0.82	0
2	MAN	K	2	3,2	11,11,12	0.59	0	15,15,17	1.14	2 (13%)
2	Z5L	L	1	2	12,13,13	0.73	1 (8%)	14,18,18	0.86	0
2	MAN	L	2	3,2	11,11,12	0.54	0	15,15,17	1.12	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	Z5L	G	1	2	-	2/4/24/24	0/1/1/1
2	MAN	G	2	3,2	-	1/2/19/22	0/1/1/1
2	Z5L	H	1	2	-	0/4/24/24	0/1/1/1
2	MAN	H	2	3,2	-	0/2/19/22	0/1/1/1
2	Z5L	I	1	2	-	2/4/24/24	0/1/1/1
2	MAN	I	2	3,2	-	0/2/19/22	0/1/1/1
2	Z5L	J	1	2	-	0/4/24/24	0/1/1/1
2	MAN	J	2	3,2	-	0/2/19/22	0/1/1/1
2	Z5L	K	1	2	-	2/4/24/24	0/1/1/1
2	MAN	K	2	3,2	-	0/2/19/22	0/1/1/1
2	Z5L	L	1	2	-	0/4/24/24	0/1/1/1
2	MAN	L	2	3,2	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	Z5L	O1-C1	2.66	1.44	1.40
2	L	1	Z5L	O1-C1	2.32	1.44	1.40
2	I	1	Z5L	O1-C1	2.26	1.44	1.40
2	J	1	Z5L	O1-C1	2.25	1.44	1.40
2	H	1	Z5L	O1-C1	2.24	1.43	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2	MAN	C1-C2-C3	3.89	115.31	109.64
2	L	2	MAN	C1-C2-C3	3.49	114.72	109.64
2	I	2	MAN	C1-C2-C3	3.46	114.68	109.64
2	J	2	MAN	C1-C2-C3	3.16	114.24	109.64
2	I	2	MAN	C1-O5-C5	3.10	116.34	112.19
2	K	2	MAN	C1-O5-C5	3.02	116.23	112.19
2	K	2	MAN	C1-C2-C3	2.53	113.33	109.64
2	G	2	MAN	C1-C2-C3	2.46	113.22	109.64
2	H	2	MAN	O5-C1-C2	2.43	116.60	110.79
2	I	1	Z5L	C3-C4-C5	-2.14	106.36	110.23

There are no chirality outliers.

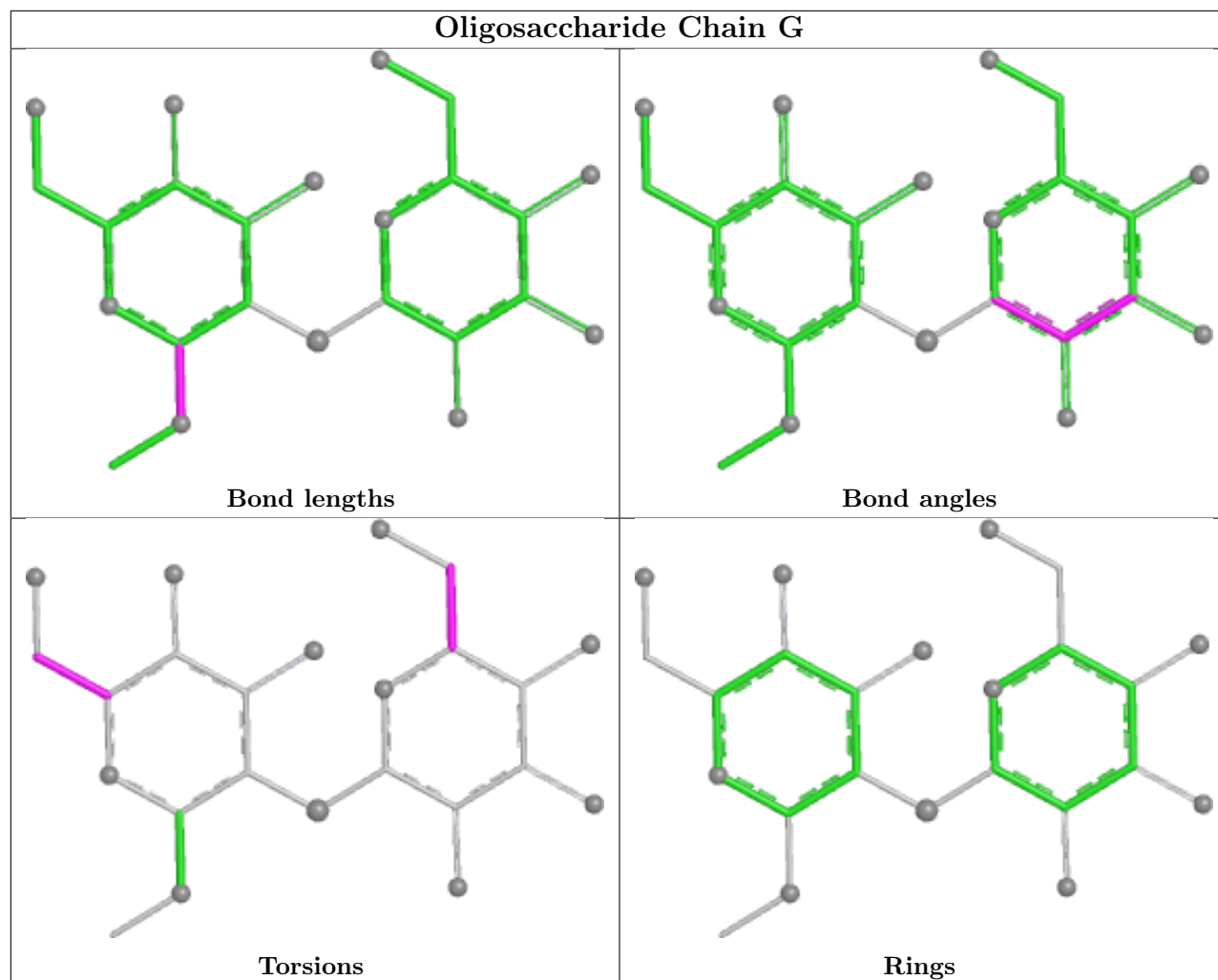
All (7) torsion outliers are listed below:

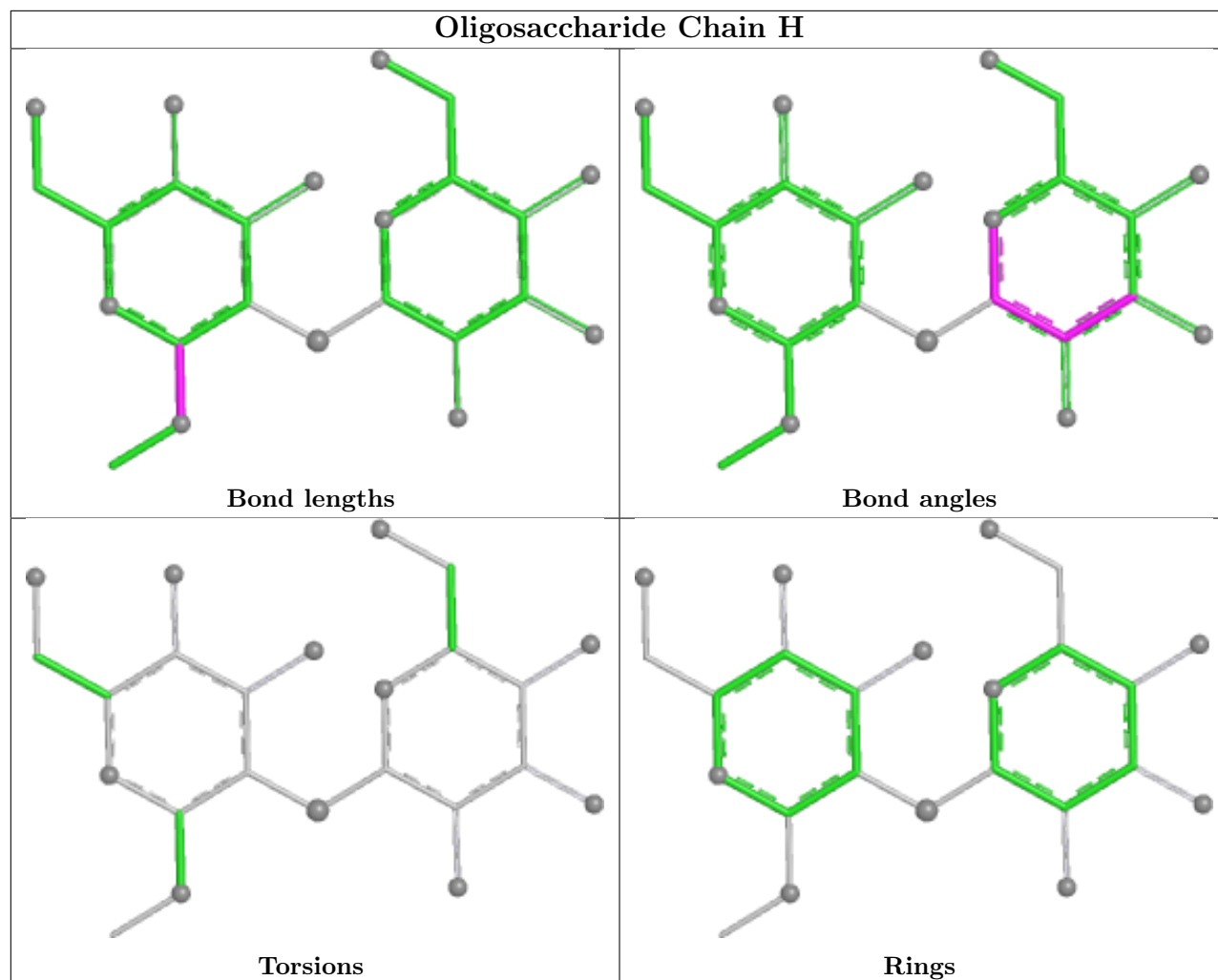
Mol	Chain	Res	Type	Atoms
2	I	1	Z5L	O5-C5-C6-O6
2	I	1	Z5L	C4-C5-C6-O6
2	K	1	Z5L	O5-C5-C6-O6
2	G	1	Z5L	O5-C5-C6-O6
2	K	1	Z5L	C4-C5-C6-O6
2	G	1	Z5L	C4-C5-C6-O6
2	G	2	MAN	O5-C5-C6-O6

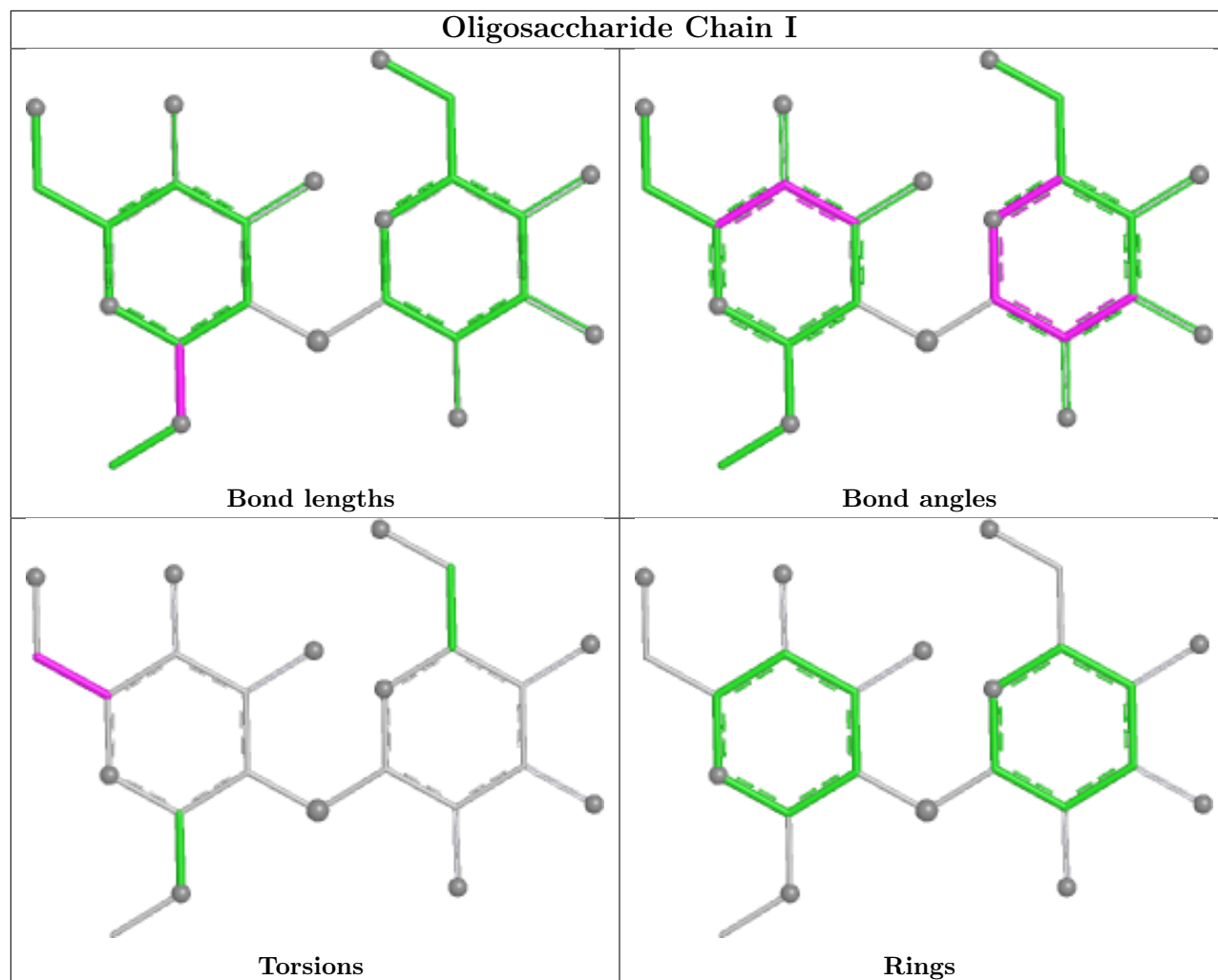
There are no ring outliers.

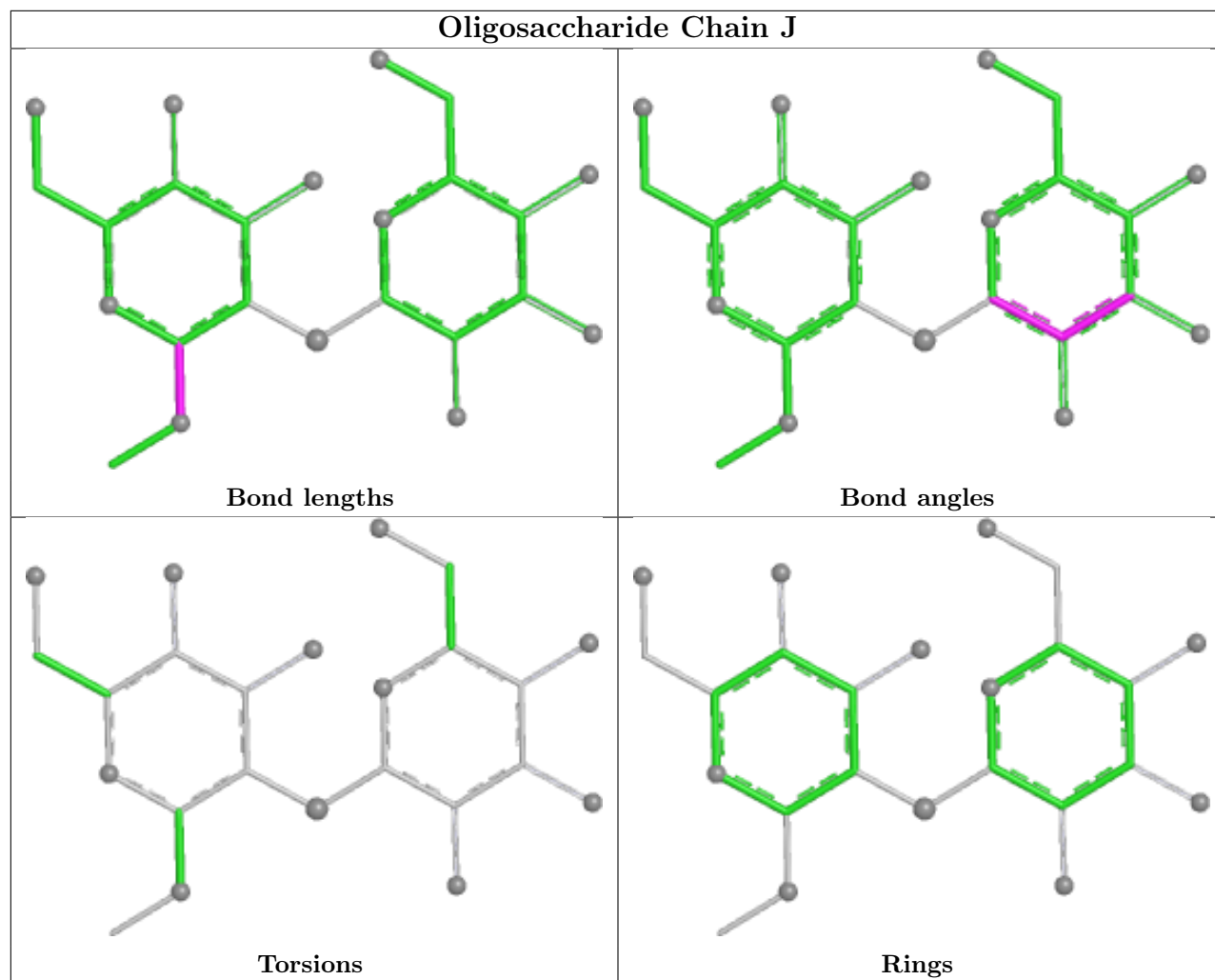
No monomer is involved in short contacts.

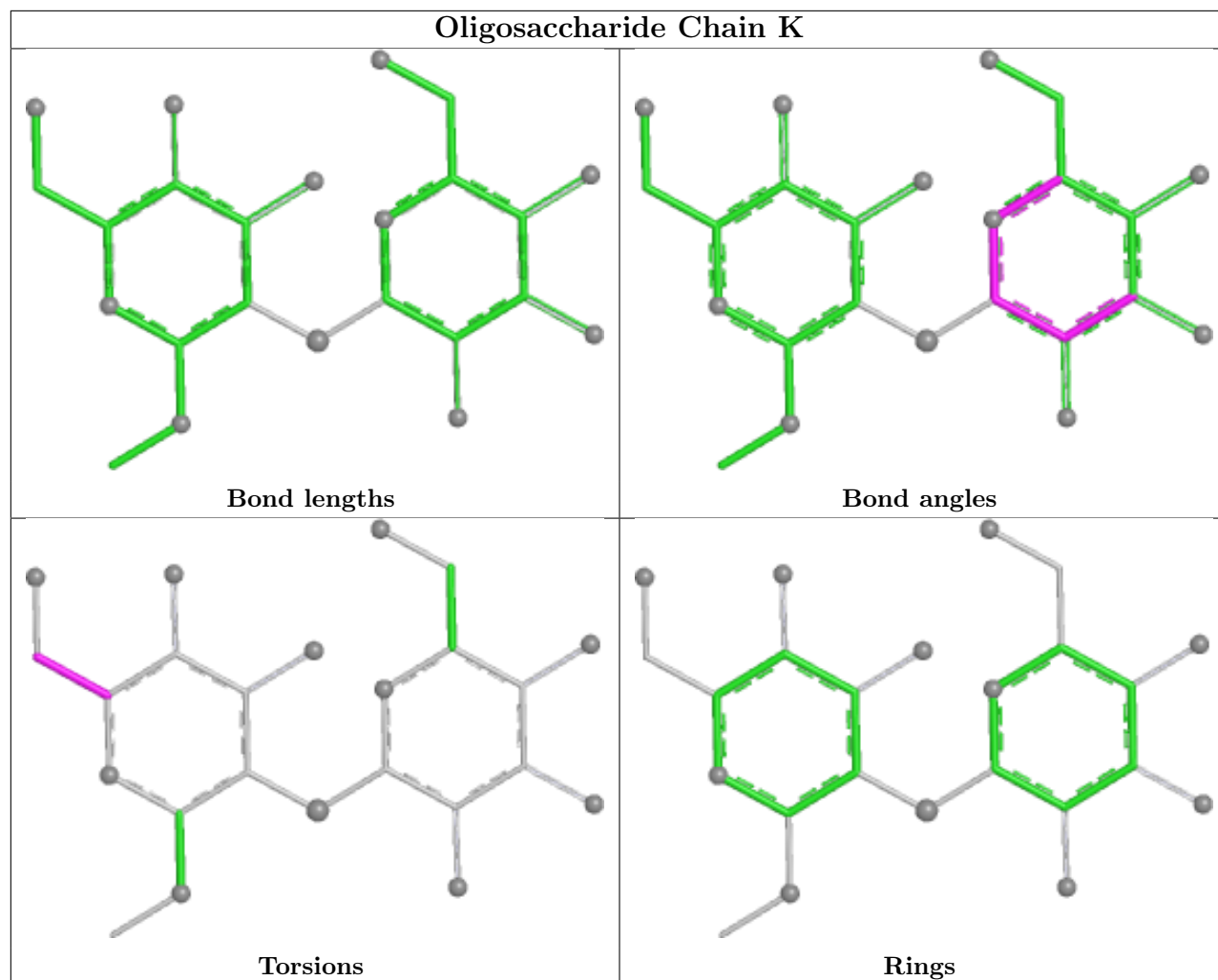
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

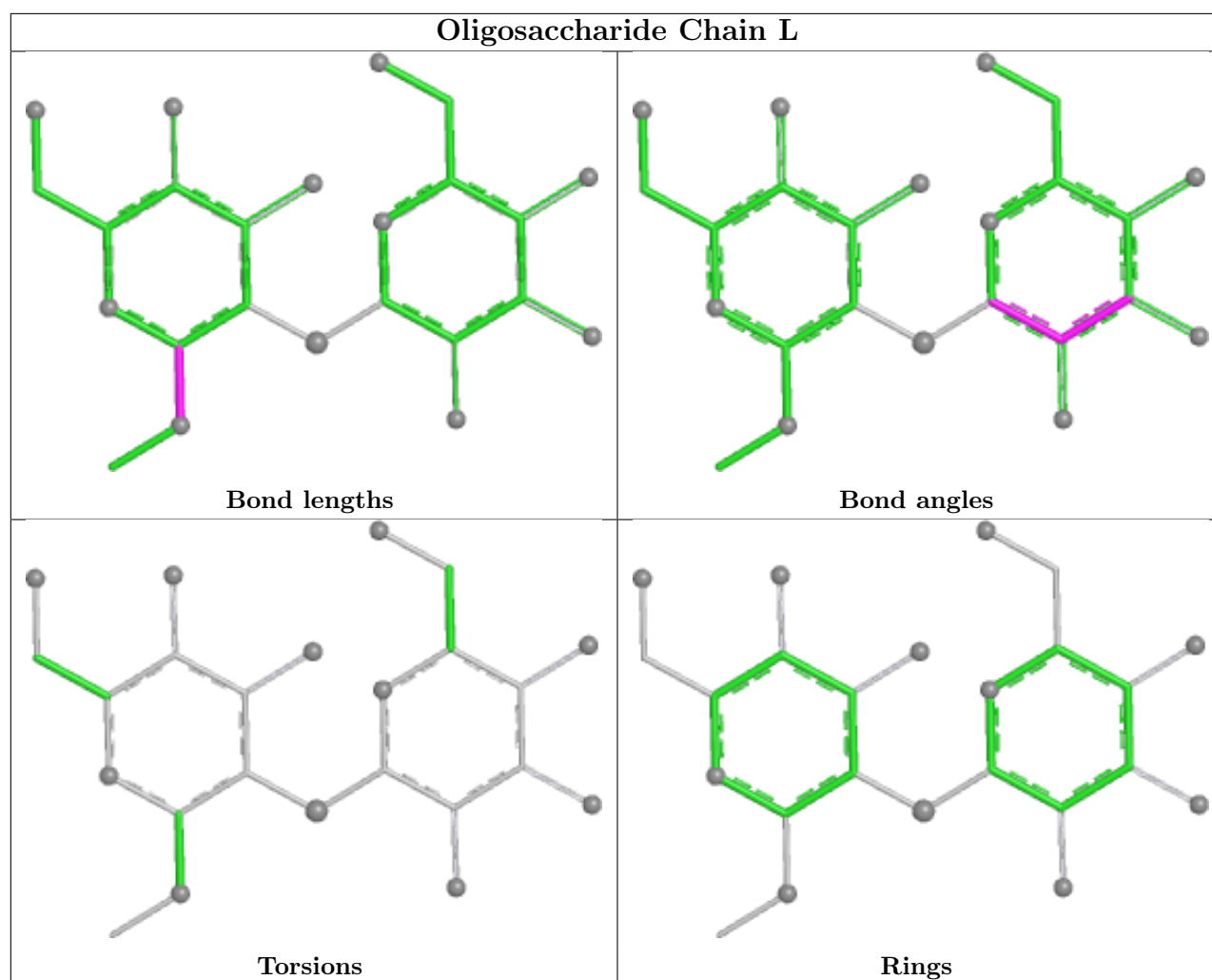












5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 for Mogul analysis.

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	$\# Z > 2$
4	GOL	C	802	-	5,5,5	0.30	0	5,5,5	0.45	0
4	GOL	E	802	-	5,5,5	0.30	0	5,5,5	0.59	0
4	GOL	A	802	-	5,5,5	0.39	0	5,5,5	0.33	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
4	GOL	C	802	-	-	2/4/4/4	-
4	GOL	E	802	-	-	4/4/4/4	-
4	GOL	A	802	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	802	GOL	O1-C1-C2-C3
4	A	802	GOL	C1-C2-C3-O3
4	A	802	GOL	O2-C2-C3-O3
4	E	802	GOL	C1-C2-C3-O3
4	C	802	GOL	O1-C1-C2-C3
4	E	802	GOL	O1-C1-C2-C3
4	A	802	GOL	O1-C1-C2-O2
4	C	802	GOL	O1-C1-C2-O2
4	E	802	GOL	O2-C2-C3-O3
4	E	802	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	736/744 (98%)	-0.24	1 (0%) 92 92	17, 23, 33, 40	0
1	B	736/744 (98%)	0.77	39 (5%) 32 34	21, 33, 44, 55	0
1	C	736/744 (98%)	-0.37	1 (0%) 92 92	15, 21, 32, 39	0
1	D	738/744 (99%)	0.24	6 (0%) 82 84	18, 28, 38, 45	0
1	E	736/744 (98%)	-0.26	1 (0%) 92 92	16, 23, 33, 40	1 (0%)
1	F	738/744 (99%)	0.13	3 (0%) 88 90	21, 30, 41, 46	0
All	All	4420/4464 (99%)	0.04	51 (1%) 76 78	15, 26, 40, 55	1 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	444	TYR	4.8
1	B	175	ILE	3.1
1	B	210	TYR	3.0
1	D	22	TRP	3.0
1	B	445	TYR	3.0
1	D	416	ILE	2.9
1	B	426	GLY	2.9
1	B	442	TYR	2.8
1	E	102	GLY	2.7
1	B	216	ASN	2.6
1	B	218	ASN	2.6
1	B	323	GLY	2.6
1	B	326	ILE	2.6
1	B	214	VAL	2.5
1	B	482	LYS	2.5
1	B	22	TRP	2.5
1	B	209	THR	2.5
1	B	319	LEU	2.5
1	B	434	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	410	GLY	2.5
1	D	199	TYR	2.4
1	B	441	GLY	2.4
1	B	199	TYR	2.4
1	B	752	PHE	2.4
1	B	417	LYS	2.3
1	B	154	PRO	2.3
1	D	321	ALA	2.3
1	B	329	SER	2.3
1	F	757	GLU	2.3
1	A	209	THR	2.3
1	B	489	SER	2.3
1	F	217	GLY	2.3
1	B	558	GLU	2.2
1	B	753	SER	2.2
1	B	424	ILE	2.2
1	C	216	ASN	2.2
1	B	406	ALA	2.2
1	F	172	ILE	2.2
1	B	184	TYR	2.2
1	B	481	LEU	2.2
1	B	732	ASP	2.2
1	D	756	LEU	2.1
1	B	725	LYS	2.1
1	B	705	SER	2.1
1	B	734	SER	2.1
1	B	446	ASN	2.0
1	B	728	THR	2.0
1	B	744	LYS	2.0
1	B	169	GLY	2.0
1	D	209	THR	2.0
1	B	420	TYR	2.0

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

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

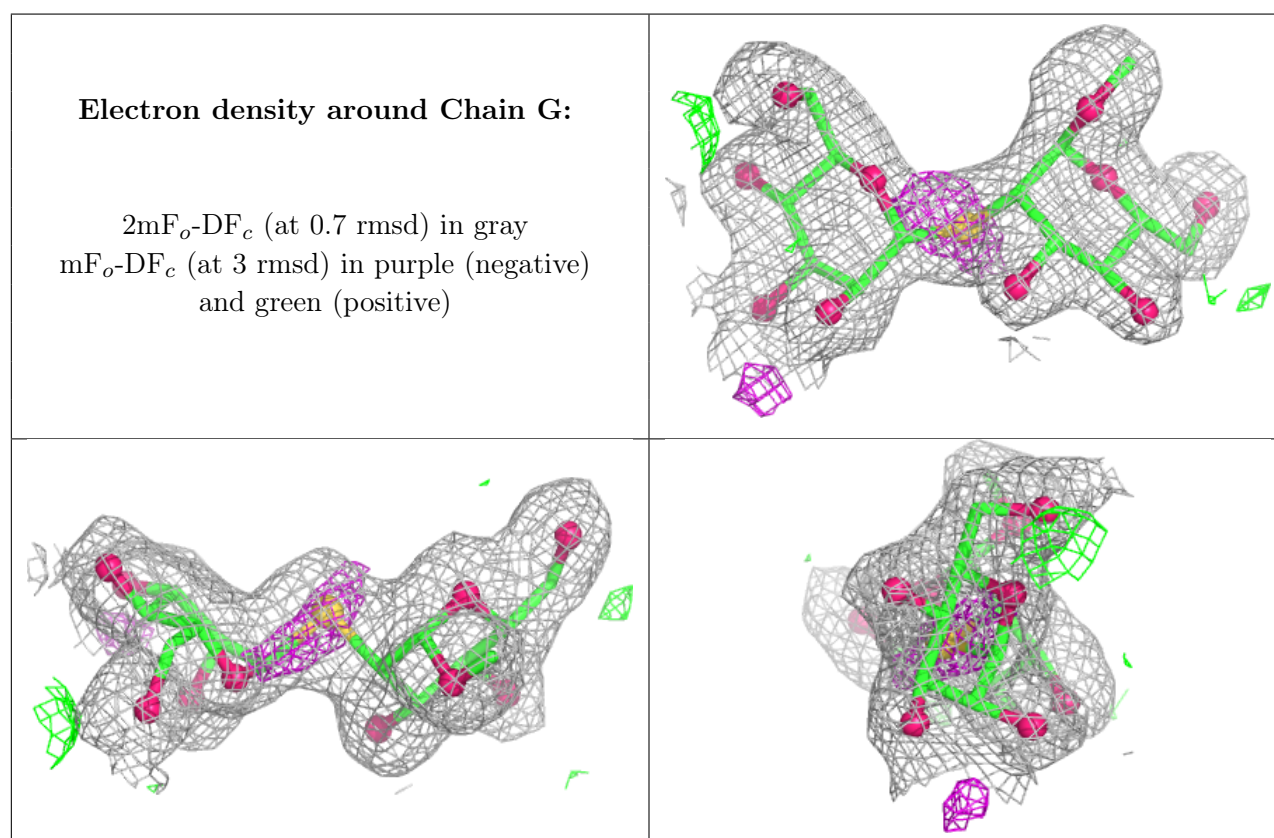
6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

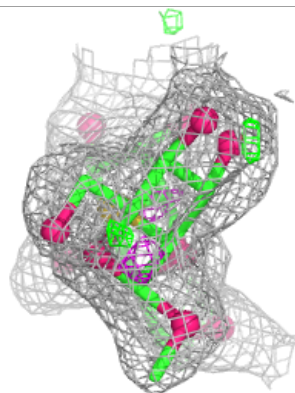
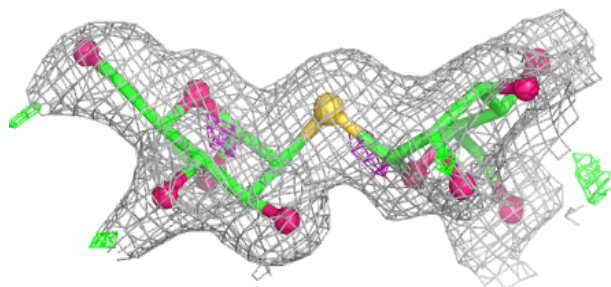
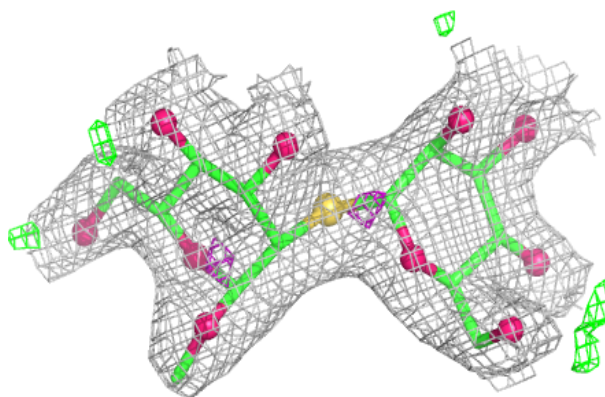
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	H	2	11/12	0.87	0.09	34,37,39,40	0
2	MAN	J	2	11/12	0.88	0.09	30,31,32,32	0
2	MAN	L	2	11/12	0.91	0.09	31,33,34,34	0
2	Z5L	H	1	13/13	0.92	0.09	36,37,39,39	0
2	Z5L	L	1	13/13	0.94	0.09	32,34,37,38	0
2	MAN	G	2	11/12	0.94	0.07	22,27,29,29	0
2	Z5L	G	1	13/13	0.95	0.07	25,27,29,31	0
2	Z5L	K	1	13/13	0.95	0.07	25,28,31,31	0
2	MAN	K	2	11/12	0.95	0.07	22,26,27,28	0
2	MAN	I	2	11/12	0.95	0.07	20,24,26,27	0
2	Z5L	J	1	13/13	0.95	0.09	28,29,34,35	0
2	Z5L	I	1	13/13	0.96	0.07	22,25,30,31	0

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

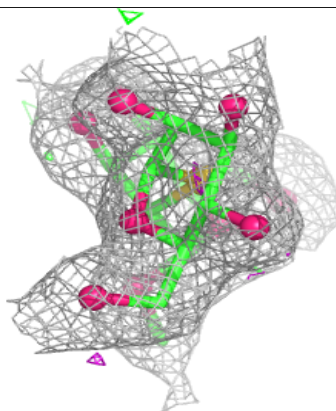
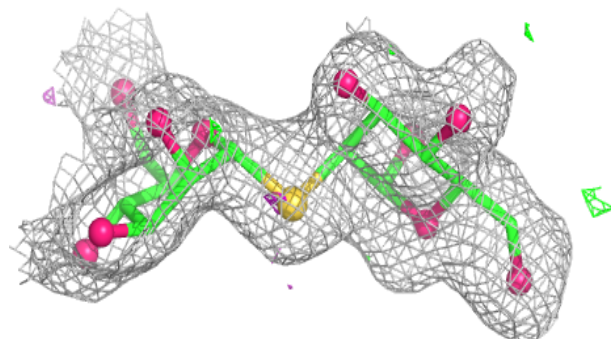
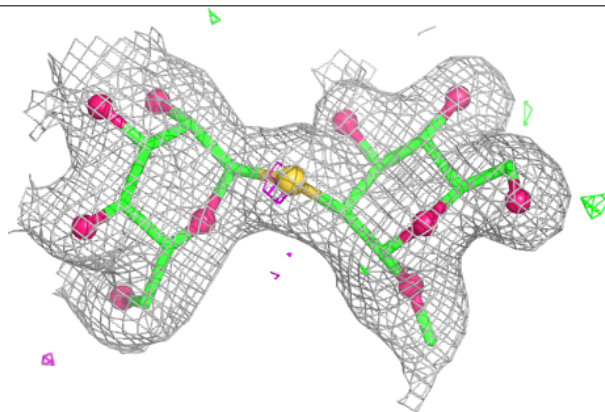


Electron density around Chain H:

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

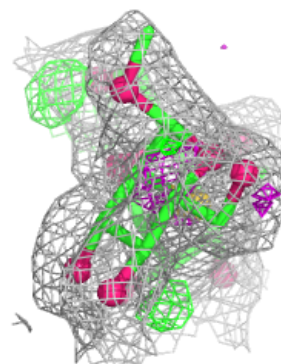
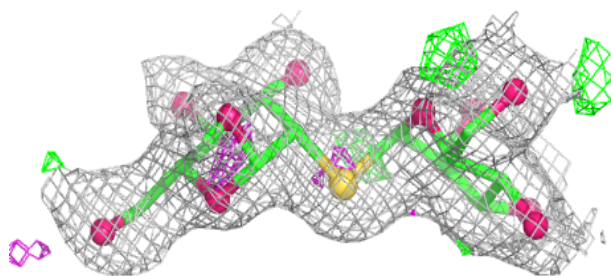
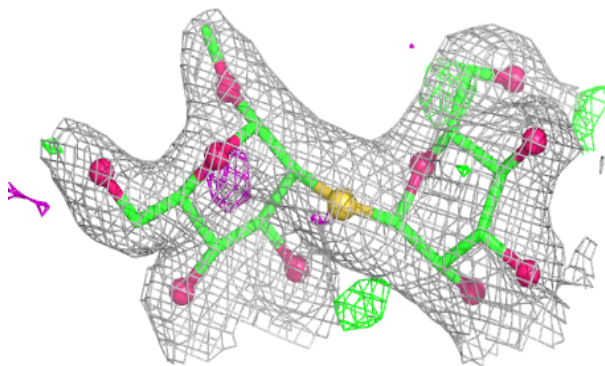
**Electron density around Chain I:**

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

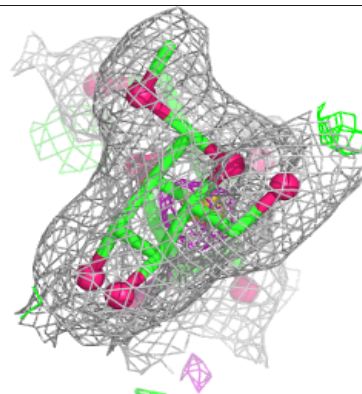
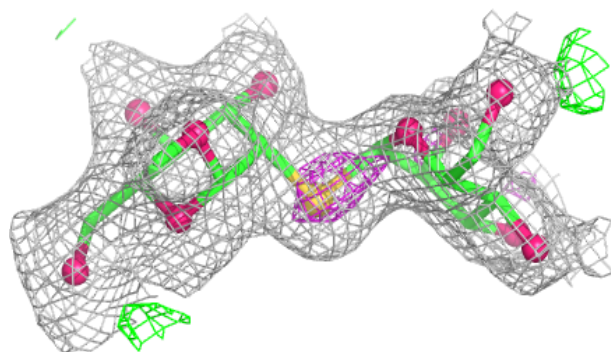
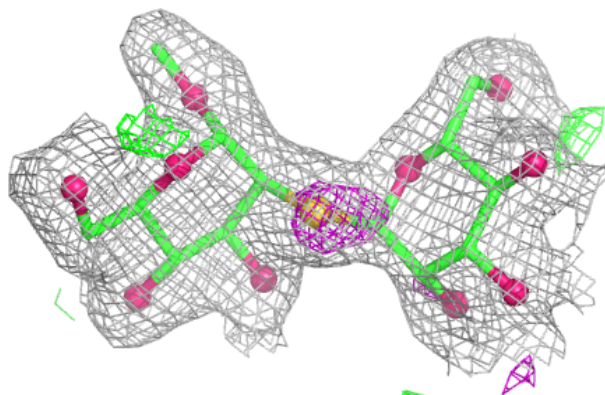


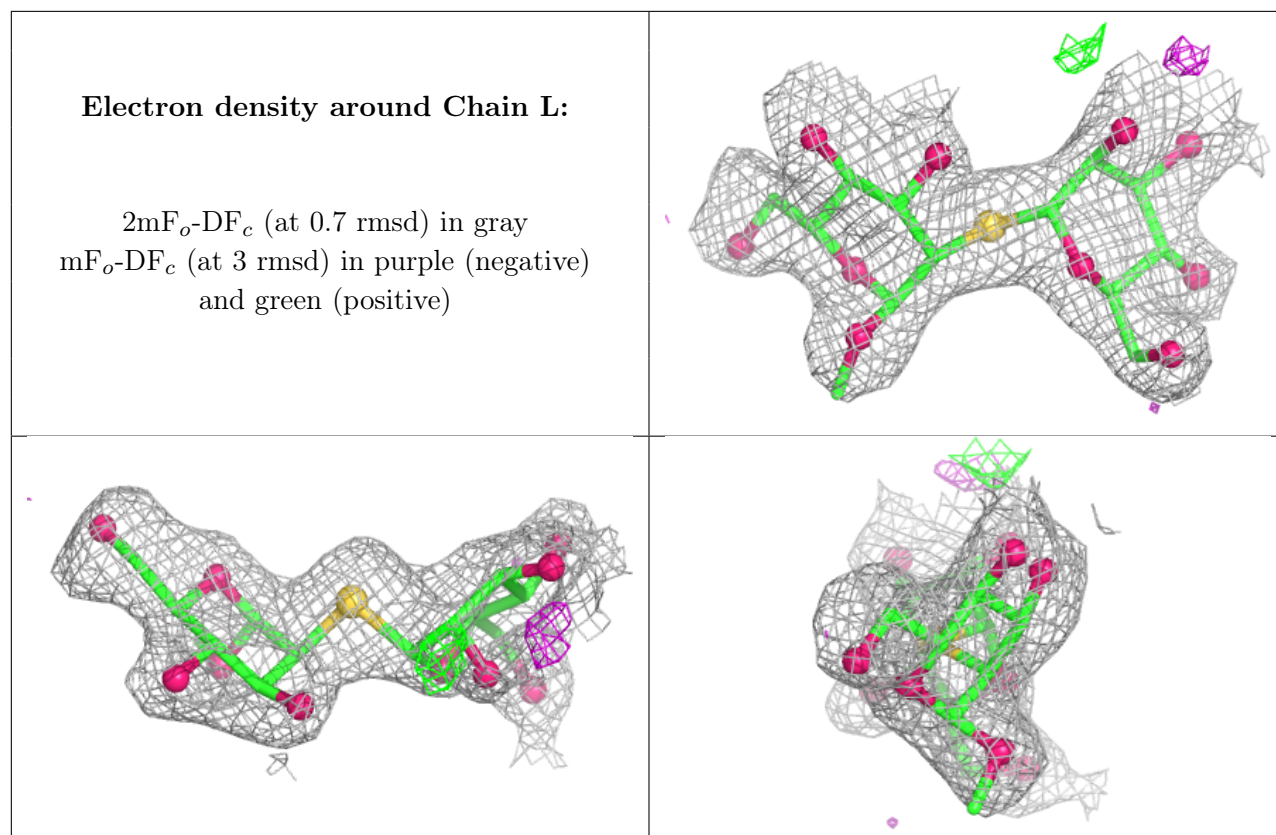
Electron density around Chain J:

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

**Electron density around Chain K:**

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	E	802	6/6	0.86	0.10	40,41,42,46	0
4	GOL	A	802	6/6	0.89	0.08	48,49,49,50	0
4	GOL	C	802	6/6	0.92	0.08	30,33,34,34	0
3	CA	B	800	1/1	0.96	0.06	36,36,36,36	0
3	CA	F	800	1/1	0.98	0.07	31,31,31,31	0
3	CA	D	800	1/1	0.98	0.04	29,29,29,29	0
3	CA	A	800	1/1	0.99	0.07	25,25,25,25	0
3	CA	E	800	1/1	0.99	0.06	24,24,24,24	0
3	CA	C	800	1/1	0.99	0.04	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.