



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 06:19 PM EST

PDB ID : 3QNQ
Title : Crystal structure of the transporter ChbC, the IIC component from the N,N'-diacetylchitobiose-specific phosphotransferase system
Authors : Cao, Y.; Jin, X.; Huang, H.; Levin, E.J.; Zhou, M.; New York Consortium on Membrane Protein Structure (NYCOMPS)
Deposited on : 2011-02-08
Resolution : 3.29 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 : 2.36
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) : 2.36

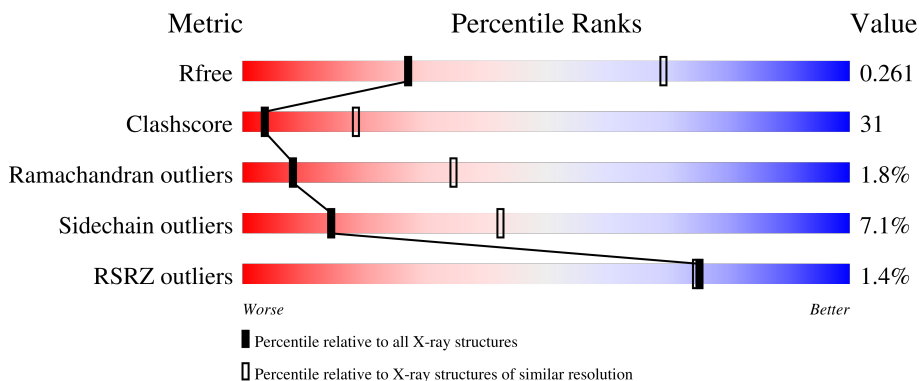
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




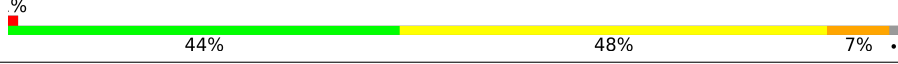
The reported resolution of this entry is 3.29 Å.

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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	442	
1	B	442	
1	C	442	
1	D	442	

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Mol	Chain	Length	Quality of chain
2	E	2	 100%
2	G	2	 100%
2	I	2	 100%
2	K	2	 100%
3	F	2	 100%
3	H	2	 100%
3	J	2	 100%
3	L	2	 100%

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 13566 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 PTS system, cellobiose-specific IIC component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	432	3272	2191	508	555	18	0	0	0
1	B	432	3288	2201	516	553	18	0	0	0
1	C	432	3280	2195	513	554	18	0	0	0
1	D	436	3307	2211	520	558	18	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	434	ALA	-	expression tag	UNP Q72XQ0
A	435	ALA	-	expression tag	UNP Q72XQ0
A	436	ALA	-	expression tag	UNP Q72XQ0
A	437	GLU	-	expression tag	UNP Q72XQ0
A	438	ASN	-	expression tag	UNP Q72XQ0
A	439	LEU	-	expression tag	UNP Q72XQ0
A	440	TYR	-	expression tag	UNP Q72XQ0
A	441	PHE	-	expression tag	UNP Q72XQ0
A	442	GLN	-	expression tag	UNP Q72XQ0
B	434	ALA	-	expression tag	UNP Q72XQ0
B	435	ALA	-	expression tag	UNP Q72XQ0
B	436	ALA	-	expression tag	UNP Q72XQ0
B	437	GLU	-	expression tag	UNP Q72XQ0
B	438	ASN	-	expression tag	UNP Q72XQ0
B	439	LEU	-	expression tag	UNP Q72XQ0
B	440	TYR	-	expression tag	UNP Q72XQ0
B	441	PHE	-	expression tag	UNP Q72XQ0
B	442	GLN	-	expression tag	UNP Q72XQ0
C	434	ALA	-	expression tag	UNP Q72XQ0
C	435	ALA	-	expression tag	UNP Q72XQ0
C	436	ALA	-	expression tag	UNP Q72XQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	437	GLU	-	expression tag	UNP Q72XQ0
C	438	ASN	-	expression tag	UNP Q72XQ0
C	439	LEU	-	expression tag	UNP Q72XQ0
C	440	TYR	-	expression tag	UNP Q72XQ0
C	441	PHE	-	expression tag	UNP Q72XQ0
C	442	GLN	-	expression tag	UNP Q72XQ0
D	434	ALA	-	expression tag	UNP Q72XQ0
D	435	ALA	-	expression tag	UNP Q72XQ0
D	436	ALA	-	expression tag	UNP Q72XQ0
D	437	GLU	-	expression tag	UNP Q72XQ0
D	438	ASN	-	expression tag	UNP Q72XQ0
D	439	LEU	-	expression tag	UNP Q72XQ0
D	440	TYR	-	expression tag	UNP Q72XQ0
D	441	PHE	-	expression tag	UNP Q72XQ0
D	442	GLN	-	expression tag	UNP Q72XQ0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	2	29	16	2	11	0	0	0
2	G	2	29	16	2	11	0	0	0
2	I	2	29	16	2	11	0	0	0
2	K	2	29	16	2	11	0	0	0

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



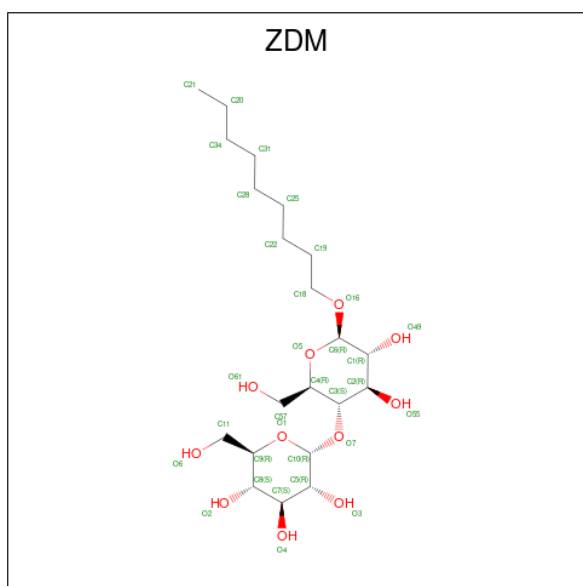
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
3	F	2	23	12	11	0	0	0

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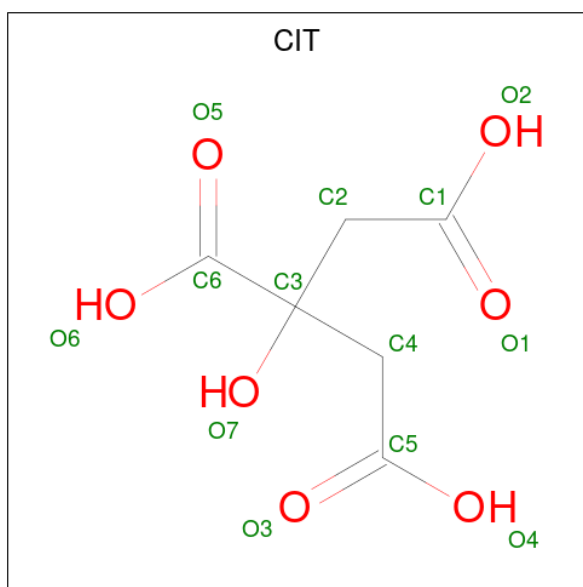
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	H	2	Total	C	O	0	0	0
			23	12	11			
3	J	2	Total	C	O	0	0	0
			23	12	11			
3	L	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 4 is nonyl 4-O-alpha-D-glucopyranosyl-beta-D-glucopyranoside (three-letter code: ZDM) (formula: C₂₁H₄₀O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			30	19	11		
4	A	1	Total	C	O	0	0
			30	19	11		
4	C	1	Total	C	O	0	0
			30	19	11		
4	C	1	Total	C	O	0	0
			30	19	11		

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).

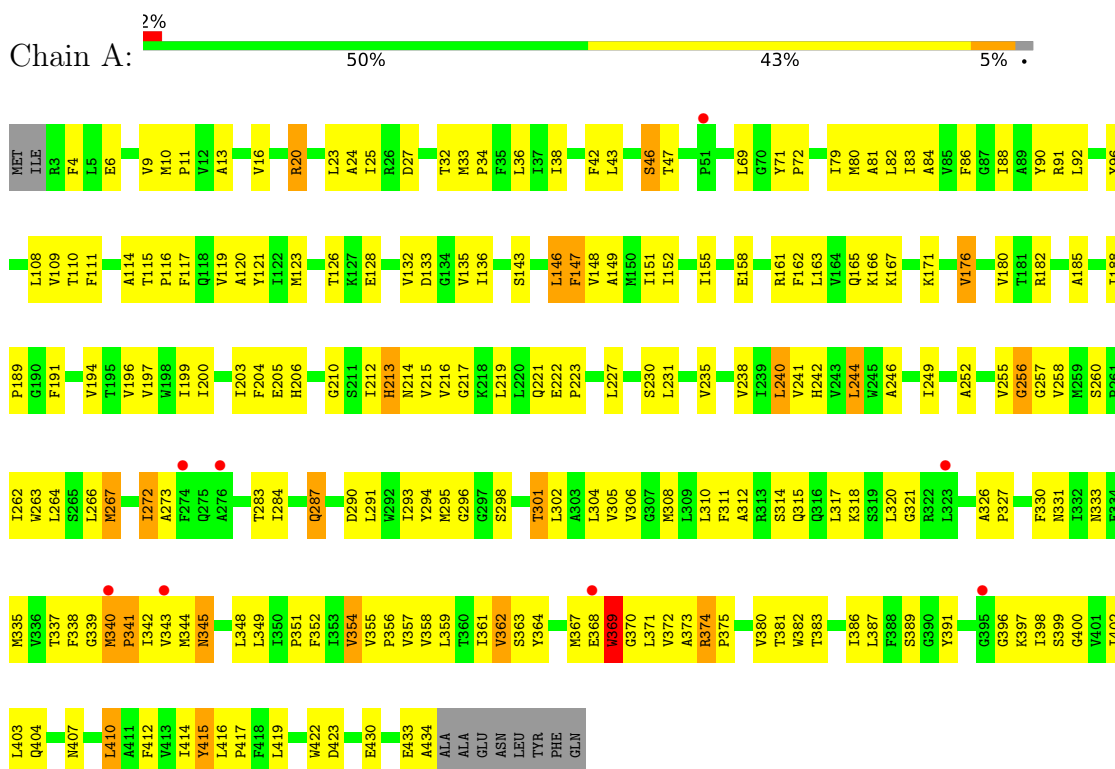


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 13 6 7	0	0
5	B	1	Total C O 13 6 7	0	0
5	B	1	Total C O 13 6 7	0	0
5	C	1	Total C O 13 6 7	0	0
5	C	1	Total C O 13 6 7	0	0
5	C	1	Total C O 13 6 7	0	0
5	D	1	Total C O 13 6 7	0	0

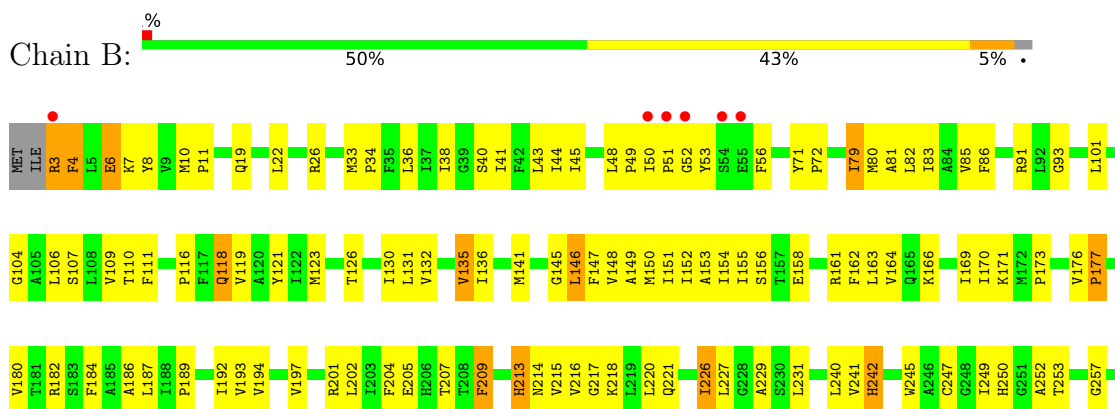
3 Residue-property plots i

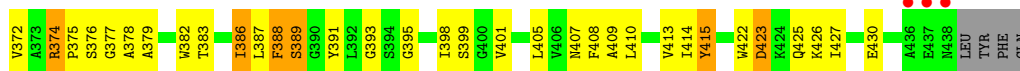
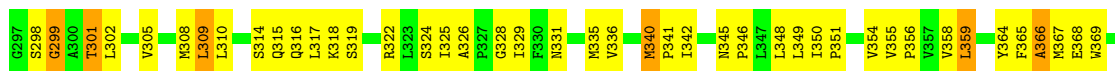
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: PTS system, cellobiose-specific IIC component



- Molecule 1: PTS system, cellobiose-specific IIC component





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

Chain E: 100%

MAG1
MAG2

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

Chain G: 100%

MAG1
MAG2

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

Chain I: 100%

MAG1
MAG2

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

Chain K: 100%

MAG1
MAG2

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

Chain F: 100%

GLC1
GLC2

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

Chain H: 100%

GLC1
GLC2

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

Chain J:  100%

GLC1
GLC2

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

Chain L:  100%

GLC1
GLC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	132.81Å 132.81Å 452.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 3.29 46.68 – 3.29	Depositor EDS
% Data completeness (in resolution range)	95.0 (19.97-3.29) 95.3 (46.68-3.29)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 3.32Å)	Xtrriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.228 , 0.264 0.228 , 0.261	Depositor DCC
R_{free} test set	3019 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	99.7	Xtrriage
Anisotropy	0.610	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13566	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CIT, GLC, ZDM, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.32	0/3356	0.53	0/4587
1	B	0.34	0/3372	0.55	1/4604 (0.0%)
1	C	0.32	0/3364	0.53	0/4596
1	D	0.34	0/3390	0.57	1/4628 (0.0%)
All	All	0.33	0/13482	0.55	2/18415 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	299	GLY	N-CA-C	-6.24	97.50	113.10
1	D	299	GLY	N-CA-C	-5.09	100.37	113.10

There are no chirality outliers.

There are no planarity outliers.

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	3272	0	3398	224	0
1	B	3288	0	3438	206	0
1	C	3280	0	3414	219	0
1	D	3307	0	3460	247	0
2	E	29	0	27	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	29	0	27	6	0
2	I	29	0	27	8	0
2	K	29	0	27	6	0
3	F	23	0	21	3	0
3	H	23	0	21	0	0
3	J	23	0	21	2	0
3	L	23	0	21	1	0
4	A	60	0	64	15	0
4	C	60	0	65	13	0
5	A	13	0	5	0	0
5	B	26	0	10	0	0
5	C	39	0	15	1	0
5	D	13	0	5	0	0
All	All	13566	0	14066	867	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 31.

All (867) 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)
4:C:600:ZDM:O49	1:D:182:ARG:HD3	1.55	1.07
1:A:367:MET:HE3	1:A:375:PRO:HD3	1.42	1.01
1:C:252:ALA:HB1	2:I:1:NAG:H5	1.45	0.98
1:C:182:ARG:HD3	4:C:443:ZDM:O49	1.63	0.98
1:B:345:ASN:ND2	1:B:348:LEU:HD12	1.83	0.93
1:D:296:GLY:HA3	1:D:302:LEU:H	1.34	0.92
1:D:324:SER:HB3	1:D:335:MET:HG2	1.51	0.90
1:C:298:SER:HB2	1:C:333:ASN:HD21	1.35	0.90
1:A:338:PHE:CD1	1:A:343:VAL:HG21	2.07	0.89
1:D:110:THR:HG22	1:D:152:ILE:HD13	1.54	0.89
1:B:164:VAL:HG12	1:B:169:ILE:HD11	1.53	0.89
1:C:111:PHE:HE1	1:C:148:VAL:HG23	1.37	0.89
1:B:4:PHE:H	1:B:4:PHE:HD2	1.21	0.88
1:A:264:LEU:HA	1:A:267:MET:HG2	1.53	0.88
1:D:173:PRO:O	1:D:176:VAL:HG12	1.74	0.86
1:C:342:ILE:HG22	1:C:342:ILE:O	1.73	0.86
1:B:345:ASN:HD21	1:B:348:LEU:HD12	1.39	0.86
1:B:295:MET:SD	1:B:386:ILE:HD11	2.16	0.85
1:C:338:PHE:CD1	1:C:343:VAL:HG21	2.12	0.85
1:D:388:PHE:H	1:D:388:PHE:HD2	1.23	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:LEU:HD23	1:D:197:VAL:HG12	1.60	0.84
1:B:82:LEU:O	1:B:85:VAL:HG12	1.79	0.82
4:A:600:ZDM:H18A	1:B:182:ARG:HD3	1.61	0.82
1:C:132:VAL:HG21	1:D:132:VAL:HG11	1.61	0.82
1:C:5:LEU:O	1:C:8:TYR:HB2	1.78	0.82
1:A:96:TYR:CD2	1:A:161:ARG:HG2	2.15	0.81
1:B:242:HIS:CD2	1:B:356:PRO:HG2	2.15	0.81
1:C:367:MET:HE3	1:C:375:PRO:HD3	1.63	0.81
1:A:298:SER:H	1:A:333:ASN:ND2	1.77	0.80
1:B:296:GLY:HA3	1:B:302:LEU:H	1.47	0.80
1:D:40:SER:O	1:D:44:ILE:HG23	1.80	0.79
1:B:52:GLY:O	1:B:56:PHE:HB2	1.83	0.78
1:D:252:ALA:HB1	2:K:1:NAG:H5	1.64	0.78
1:C:337:THR:O	1:C:343:VAL:HG23	1.84	0.78
1:A:244:LEU:HD23	1:A:249:ILE:HB	1.67	0.76
1:D:267:MET:HG3	1:D:287:GLN:HE22	1.49	0.76
1:B:50:ILE:HG23	1:B:51:PRO:HD2	1.67	0.76
1:D:50:ILE:HB	1:D:53:TYR:HB3	1.66	0.76
1:B:217:GLY:HA2	1:B:221:GLN:HB3	1.66	0.76
1:C:161:ARG:HD2	1:C:162:PHE:N	2.01	0.76
1:A:308:MET:O	1:A:312:ALA:HB2	1.86	0.75
1:D:267:MET:HG3	1:D:287:GLN:NE2	2.01	0.75
1:C:19:GLN:HG3	1:C:22:LEU:HB2	1.69	0.75
1:C:38:ILE:HG21	1:D:194:VAL:HG21	1.68	0.75
1:D:367:MET:CE	1:D:375:PRO:HD3	2.17	0.74
1:D:242:HIS:CD2	1:D:356:PRO:HG2	2.22	0.74
1:D:266:LEU:HD12	1:D:284:ILE:HG22	1.69	0.74
1:D:287:GLN:H	1:D:287:GLN:CD	1.91	0.73
1:C:96:TYR:CD2	1:C:161:ARG:HG2	2.23	0.73
1:C:317:LEU:HD11	1:C:422:TRP:HD1	1.52	0.73
1:B:19:GLN:HG2	1:B:22:LEU:HD13	1.71	0.73
1:B:176:VAL:HG23	2:E:2:NAG:H62	1.70	0.73
1:C:298:SER:H	1:C:333:ASN:ND2	1.86	0.73
1:D:340:MET:HG2	1:D:348:LEU:HD12	1.70	0.73
1:C:27:ASP:HB3	4:C:600:ZDM:O61	1.88	0.73
1:A:126:THR:HG23	1:A:128:GLU:HB2	1.68	0.73
1:D:231:LEU:HD13	1:D:364:TYR:CD1	2.23	0.73
1:A:182:ARG:HD2	4:A:443:ZDM:O49	1.88	0.73
1:B:367:MET:HE1	1:B:375:PRO:HD3	1.71	0.73
1:C:9:VAL:C	1:C:11:PRO:HD2	2.08	0.73
1:B:367:MET:CE	1:B:375:PRO:HD3	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:443:ZDM:H31	1:B:34:PRO:HG2	1.70	0.72
1:C:136:ILE:HB	1:D:136:ILE:HB	1.70	0.72
1:A:182:ARG:HH11	4:A:443:ZDM:H6	1.53	0.72
1:B:359:LEU:HD22	1:B:407:ASN:HB3	1.71	0.72
1:C:296:GLY:O	1:C:331:ASN:HA	1.89	0.72
1:D:324:SER:HB3	1:D:335:MET:CG	2.20	0.72
1:A:111:PHE:HE1	1:A:148:VAL:HG22	1.53	0.71
1:C:111:PHE:CE1	1:C:148:VAL:HG23	2.24	0.71
1:D:358:VAL:HG12	1:D:358:VAL:O	1.90	0.71
1:B:36:LEU:HD21	1:B:80:MET:HG2	1.72	0.71
1:B:204:PHE:HE1	1:B:215:VAL:HG21	1.55	0.71
1:A:79:ILE:HG22	1:A:79:ILE:O	1.91	0.71
1:A:80:MET:HE2	1:A:143:SER:HA	1.73	0.70
1:A:182:ARG:NH1	4:A:443:ZDM:H6	2.06	0.70
1:C:269:GLN:HE21	1:C:282:ASN:HD21	1.39	0.70
1:C:345:ASN:HD21	1:C:348:LEU:H	1.36	0.70
1:D:367:MET:HE1	1:D:375:PRO:HD3	1.74	0.70
1:A:337:THR:O	1:A:343:VAL:HG23	1.90	0.70
1:D:111:PHE:HE1	1:D:148:VAL:HG22	1.56	0.70
1:B:173:PRO:O	1:B:176:VAL:HG12	1.91	0.69
1:D:388:PHE:N	1:D:388:PHE:CD2	2.60	0.69
1:D:231:LEU:HD13	1:D:364:TYR:CG	2.27	0.69
1:A:387:LEU:HA	1:A:404:GLN:HE22	1.56	0.69
1:B:130:ILE:HD11	1:C:130:ILE:HD13	1.73	0.69
1:C:213:HIS:HD2	1:C:214:ASN:H	1.40	0.69
4:C:600:ZDM:O49	1:D:182:ARG:CD	2.37	0.69
1:B:71:TYR:HB2	1:B:72:PRO:HD3	1.75	0.69
1:C:148:VAL:HG12	1:C:216:VAL:HG21	1.73	0.69
1:A:13:ALA:O	1:A:16:VAL:HG12	1.93	0.68
1:A:96:TYR:HD2	1:A:161:ARG:HG2	1.55	0.68
1:B:151:ILE:O	1:B:155:ILE:HG13	1.92	0.68
1:A:27:ASP:HB3	4:A:600:ZDM:O61	1.94	0.68
1:B:250:HIS:CE1	1:B:253:THR:HG23	2.28	0.68
1:D:376:SER:HB3	1:D:395:GLY:N	2.08	0.68
1:C:86:PHE:CE2	1:D:86:PHE:CZ	2.81	0.68
1:A:295:MET:SD	1:A:386:ILE:HD11	2.34	0.68
1:C:204:PHE:CD1	1:C:215:VAL:HG21	2.29	0.68
1:C:182:ARG:CD	4:C:443:ZDM:O49	2.39	0.68
1:D:146:LEU:HD11	1:D:264:LEU:HD11	1.75	0.68
1:A:136:ILE:HB	1:B:136:ILE:HB	1.75	0.68
1:D:299:GLY:C	1:D:301:THR:H	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:SER:HB3	1:C:352:PHE:CZ	2.29	0.68
1:A:345:ASN:HD21	1:A:348:LEU:H	1.40	0.68
1:A:182:ARG:CD	4:A:443:ZDM:O49	2.42	0.67
1:B:296:GLY:HA2	1:B:302:LEU:HB2	1.76	0.67
1:A:351:PRO:HB2	1:A:415:TYR:CE1	2.30	0.67
1:C:342:ILE:O	1:C:342:ILE:CG2	2.43	0.67
1:D:345:ASN:O	1:D:349:LEU:HB2	1.94	0.67
1:A:264:LEU:HA	1:A:267:MET:CG	2.25	0.67
1:B:410:LEU:O	1:B:414:ILE:HG13	1.95	0.67
1:B:176:VAL:HG21	1:B:180:VAL:HG11	1.77	0.67
1:C:213:HIS:CD2	1:C:214:ASN:N	2.62	0.67
1:A:213:HIS:HD2	1:A:214:ASN:N	1.93	0.67
1:B:204:PHE:HA	1:B:207:THR:HG23	1.76	0.67
1:A:246:ALA:HB1	1:A:349:LEU:HD21	1.77	0.66
1:B:110:THR:HG23	1:B:197:VAL:HG11	1.77	0.66
1:A:301:THR:HG21	1:A:333:ASN:HB2	1.77	0.66
1:D:382:TRP:CZ3	1:D:383:THR:HG22	2.31	0.66
1:C:204:PHE:CE1	1:C:215:VAL:HG11	2.30	0.66
1:C:242:HIS:NE2	1:C:298:SER:O	2.29	0.66
1:B:4:PHE:N	1:B:4:PHE:CD2	2.59	0.66
1:B:33:MET:HB2	1:B:34:PRO:HD3	1.78	0.66
1:B:296:GLY:HA3	1:B:302:LEU:N	2.10	0.66
1:C:345:ASN:O	1:C:349:LEU:HB2	1.96	0.66
1:D:116:PRO:O	1:D:117:PHE:HB2	1.96	0.66
1:A:345:ASN:O	1:A:349:LEU:HB2	1.94	0.65
1:A:80:MET:CE	1:A:143:SER:HA	2.25	0.65
1:A:260:SER:O	1:A:264:LEU:HG	1.95	0.65
1:C:34:PRO:HA	1:C:37:ILE:HD12	1.77	0.65
1:C:188:ILE:HB	1:C:189:PRO:HD3	1.79	0.65
1:A:119:VAL:HG22	1:A:132:VAL:HB	1.78	0.65
1:B:252:ALA:HB1	2:G:1:NAG:H5	1.78	0.65
1:C:316:GLN:HE22	1:C:426:LYS:HD2	1.61	0.65
1:C:381:THR:C	1:C:383:THR:H	2.00	0.65
1:B:213:HIS:CD2	1:B:214:ASN:N	2.64	0.65
1:A:33:MET:HB2	1:A:34:PRO:HD3	1.80	0.64
1:C:110:THR:HG23	1:C:197:VAL:HG11	1.78	0.64
1:A:296:GLY:HA3	1:A:302:LEU:H	1.62	0.64
1:A:252:ALA:HB1	2:E:1:NAG:H5	1.79	0.64
1:D:316:GLN:HG3	1:D:430:GLU:OE2	1.98	0.64
1:C:41:ILE:HD12	1:D:191:PHE:CE1	2.32	0.64
1:C:412:PHE:HE2	1:C:416:LEU:HD22	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:THR:CG2	1:A:128:GLU:HB2	2.27	0.63
1:A:235:VAL:HA	1:A:238:VAL:HG12	1.79	0.63
1:C:191:PHE:CE1	1:D:41:ILE:HD12	2.34	0.63
1:D:36:LEU:HD21	1:D:80:MET:HG2	1.79	0.63
1:A:109:VAL:CG2	1:B:83:ILE:HD11	2.29	0.63
1:B:296:GLY:O	1:B:331:ASN:HA	1.99	0.63
1:C:38:ILE:CG2	1:D:194:VAL:HG21	2.28	0.63
1:D:43:LEU:HD12	1:D:378:ALA:HB2	1.80	0.63
1:D:296:GLY:HA3	1:D:302:LEU:N	2.10	0.63
1:D:55:GLU:HA	1:D:58:ALA:HB3	1.79	0.62
1:A:71:TYR:HB2	1:A:72:PRO:HD3	1.81	0.62
1:D:89:ALA:HB3	1:D:104:GLY:HA2	1.80	0.62
4:A:600:ZDM:O49	1:B:182:ARG:HD3	1.99	0.62
1:D:358:VAL:O	1:D:359:LEU:HD23	1.99	0.62
1:A:46:SER:HB3	1:A:69:LEU:HD12	1.82	0.62
1:B:10:MET:HG3	1:B:247:CYS:HB3	1.82	0.62
1:C:340:MET:HG2	1:C:342:ILE:HG13	1.79	0.62
1:D:267:MET:SD	1:D:379:ALA:HB2	2.40	0.62
1:C:295:MET:HG2	1:C:386:ILE:CD1	2.30	0.62
1:B:249:ILE:HG22	1:B:250:HIS:H	1.65	0.62
1:A:110:THR:CG2	1:A:197:VAL:HG21	2.30	0.62
1:B:130:ILE:HG21	1:D:132:VAL:HG12	1.80	0.62
1:C:410:LEU:O	1:C:414:ILE:HG13	1.99	0.62
4:C:443:ZDM:H28A	1:D:34:PRO:HG2	1.81	0.62
1:C:211:SER:HB2	1:C:213:HIS:CD2	2.34	0.61
1:D:103:SER:HB2	1:D:157:THR:HG23	1.80	0.61
1:D:296:GLY:O	1:D:331:ASN:HA	2.00	0.61
1:A:188:ILE:HB	1:A:189:PRO:HD3	1.80	0.61
1:B:26:ARG:HG3	1:B:257:GLY:HA3	1.82	0.61
1:A:135:VAL:HB	1:B:135:VAL:HG22	1.83	0.61
1:C:253:THR:HG22	2:I:1:NAG:H1	1.81	0.61
1:D:252:ALA:HB2	2:K:2:NAG:C7	2.30	0.61
1:D:295:MET:HE1	1:D:407:ASN:HB2	1.81	0.61
1:C:351:PRO:HB2	1:C:415:TYR:CD1	2.35	0.61
4:C:600:ZDM:HO49	1:D:182:ARG:HD3	1.61	0.61
1:D:71:TYR:HB2	1:D:72:PRO:HD3	1.82	0.61
1:A:123:MET:O	1:A:126:THR:HG22	2.00	0.61
1:C:250:HIS:CE1	1:C:253:THR:HG23	2.36	0.61
1:A:369:TRP:HB2	1:A:371:LEU:HD12	1.82	0.61
1:B:202:LEU:O	1:B:205:GLU:HB3	2.00	0.61
1:C:254:ILE:O	1:C:258:VAL:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:LEU:HD12	1:B:131:LEU:O	2.01	0.61
1:B:264:LEU:HA	1:B:267:MET:HB3	1.83	0.61
1:B:331:ASN:N	1:B:331:ASN:HD22	1.98	0.61
1:D:33:MET:HB2	1:D:34:PRO:HD3	1.83	0.61
1:C:298:SER:CB	1:C:333:ASN:HD21	2.12	0.61
1:B:80:MET:HE1	1:B:264:LEU:HD13	1.83	0.61
1:A:362:VAL:HG12	1:A:362:VAL:O	2.00	0.60
1:C:252:ALA:HB2	2:I:2:NAG:C7	2.31	0.60
1:B:43:LEU:HD12	1:B:44:ILE:HG22	1.83	0.60
1:D:204:PHE:HA	1:D:207:THR:HG23	1.82	0.60
1:D:359:LEU:CD1	1:D:407:ASN:HB3	2.30	0.60
1:A:110:THR:HG21	1:A:197:VAL:HG21	1.84	0.60
1:C:408:PHE:CG	1:C:408:PHE:O	2.54	0.60
1:C:33:MET:HB2	1:C:34:PRO:HD3	1.84	0.60
1:A:126:THR:HG23	1:A:128:GLU:H	1.66	0.60
4:C:443:ZDM:O55	4:C:443:ZDM:H5	2.02	0.60
1:B:204:PHE:CE1	1:B:215:VAL:HG21	2.37	0.60
1:D:188:ILE:HB	1:D:189:PRO:HD3	1.84	0.60
1:A:91:ARG:HE	4:A:600:ZDM:C57	2.14	0.60
1:D:147:PHE:O	1:D:151:ILE:HG13	2.02	0.60
1:D:172:MET:HG3	1:D:176:VAL:HG11	1.82	0.60
1:D:249:ILE:HG22	1:D:250:HIS:N	2.16	0.60
1:B:252:ALA:HB2	2:G:2:NAG:C7	2.32	0.59
1:A:298:SER:CB	1:A:333:ASN:HD21	2.14	0.59
1:A:86:PHE:CE2	1:B:86:PHE:CZ	2.90	0.59
1:A:338:PHE:CE1	1:A:343:VAL:HG21	2.36	0.59
1:C:147:PHE:HA	1:C:150:MET:HE3	1.84	0.59
1:A:146:LEU:HD21	1:A:264:LEU:HD11	1.83	0.59
1:A:38:ILE:HG21	1:B:194:VAL:HG21	1.84	0.59
1:C:79:ILE:CD1	1:D:112:LEU:HD12	2.33	0.59
1:D:364:TYR:CE2	1:D:368:GLU:HG3	2.38	0.59
1:B:34:PRO:O	1:B:38:ILE:HG13	2.02	0.59
1:B:216:VAL:O	1:B:220:LEU:HB2	2.02	0.59
1:D:41:ILE:O	1:D:44:ILE:HG13	2.02	0.59
1:D:293:ILE:N	1:D:293:ILE:HD12	2.18	0.59
1:A:359:LEU:HD22	1:A:407:ASN:OD1	2.03	0.58
1:B:382:TRP:CZ3	1:B:383:THR:HG22	2.38	0.58
1:C:79:ILE:HD11	1:D:112:LEU:CD1	2.33	0.58
1:B:249:ILE:HG22	1:B:250:HIS:N	2.17	0.58
1:B:325:ILE:HD12	1:B:326:ALA:N	2.18	0.58
1:D:260:SER:O	1:D:264:LEU:HG	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1:GLC:O3	3:F:2:GLC:O5	2.20	0.58
1:A:317:LEU:HD11	1:A:422:TRP:HD1	1.66	0.58
1:B:359:LEU:HD22	1:B:407:ASN:CB	2.33	0.58
1:D:409:ALA:O	1:D:413:VAL:HG13	2.03	0.58
1:B:130:ILE:CD1	1:C:130:ILE:HD13	2.32	0.58
1:D:110:THR:HG23	1:D:197:VAL:HG21	1.85	0.58
1:C:91:ARG:HE	4:C:600:ZDM:H57A	1.67	0.58
1:A:304:LEU:HB2	1:A:415:TYR:CD2	2.39	0.58
1:A:351:PRO:HB2	1:A:415:TYR:CD1	2.38	0.58
1:A:416:LEU:N	1:A:417:PRO:HD2	2.19	0.58
4:A:443:ZDM:C57	1:B:91:ARG:HE	2.17	0.58
1:B:268:ASP:OD1	1:B:271:ARG:HD3	2.04	0.58
1:C:86:PHE:CZ	1:D:86:PHE:CZ	2.92	0.58
1:C:213:HIS:HD2	1:C:214:ASN:N	2.01	0.58
1:C:71:TYR:HB2	1:C:72:PRO:HD3	1.84	0.58
1:C:283:THR:HA	1:C:374:ARG:HG3	1.86	0.58
1:D:50:ILE:HB	1:D:53:TYR:CB	2.34	0.58
1:B:296:GLY:CA	1:B:302:LEU:HB2	2.34	0.58
1:A:298:SER:HB2	1:A:333:ASN:HD21	1.69	0.57
1:B:335:MET:CE	1:B:335:MET:HA	2.34	0.57
1:C:182:ARG:NH1	4:C:443:ZDM:H6	2.19	0.57
1:A:42:PHE:CD1	1:A:72:PRO:HG2	2.39	0.57
1:B:119:VAL:HG22	1:B:135:VAL:HG11	1.86	0.57
1:B:353:ILE:O	1:B:356:PRO:HD2	2.04	0.57
1:A:146:LEU:HD21	1:A:264:LEU:CD1	2.34	0.57
1:A:295:MET:HE1	1:A:407:ASN:HB3	1.86	0.57
1:B:340:MET:N	1:B:341:PRO:HA	2.20	0.57
1:B:299:GLY:C	1:B:301:THR:H	2.08	0.57
1:C:268:ASP:O	1:C:271:ARG:HB3	2.04	0.57
1:D:386:ILE:HG23	1:D:387:LEU:N	2.19	0.57
4:A:443:ZDM:H5	4:A:443:ZDM:O55	2.04	0.57
1:B:282:ASN:O	1:B:374:ARG:HG2	2.04	0.57
1:C:351:PRO:HB2	1:C:415:TYR:CE1	2.40	0.57
1:C:369:TRP:HB3	1:C:371:LEU:HD12	1.86	0.57
1:A:204:PHE:CE1	1:A:215:VAL:HG11	2.40	0.57
1:A:295:MET:CE	1:A:407:ASN:HB3	2.35	0.57
1:C:10:MET:N	1:C:11:PRO:HD2	2.20	0.57
1:D:367:MET:CE	1:D:374:ARG:HA	2.35	0.57
1:A:311:PHE:N	1:A:311:PHE:CD2	2.72	0.57
1:D:53:TYR:HA	1:D:56:PHE:HB3	1.87	0.57
1:D:85:VAL:CG1	1:D:107:SER:HB3	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:HIS:CE1	1:D:253:THR:HG23	2.40	0.56
1:A:80:MET:HE3	1:A:146:LEU:HD23	1.86	0.56
1:A:291:LEU:HD22	1:A:389:SER:OG	2.05	0.56
1:A:382:TRP:CZ3	1:A:383:THR:HG22	2.40	0.56
1:C:217:GLY:HA2	1:C:221:GLN:HB3	1.86	0.56
1:A:213:HIS:CD2	1:A:214:ASN:N	2.71	0.56
1:A:252:ALA:CB	2:E:1:NAG:H5	2.36	0.56
1:A:310:LEU:C	1:A:311:PHE:HD2	2.08	0.56
1:D:249:ILE:HG22	1:D:250:HIS:H	1.71	0.56
1:A:311:PHE:HE1	1:A:416:LEU:HD21	1.71	0.56
1:A:221:GLN:O	1:A:221:GLN:HG3	2.03	0.56
1:B:146:LEU:HA	1:B:149:ALA:HB3	1.88	0.56
1:D:250:HIS:ND1	1:D:253:THR:HG23	2.21	0.56
1:B:287:GLN:HA	1:B:290:ASP:HB2	1.87	0.56
1:C:331:ASN:N	1:C:331:ASN:HD22	2.04	0.56
1:D:119:VAL:HG23	1:D:132:VAL:CG2	2.36	0.56
1:D:221:GLN:O	1:D:225:SER:HB2	2.05	0.56
1:A:20:ARG:HH11	1:A:20:ARG:HB3	1.71	0.56
1:B:44:ILE:O	1:B:44:ILE:HG13	2.05	0.56
1:C:110:THR:CG2	1:C:197:VAL:HG11	2.36	0.56
1:A:382:TRP:HE1	2:E:1:NAG:HN2	1.54	0.56
1:A:315:GLN:HB2	1:A:430:GLU:OE1	2.07	0.55
1:A:372:VAL:HG13	1:A:399:SER:O	2.07	0.55
1:B:367:MET:HB3	1:B:374:ARG:HD2	1.88	0.55
1:A:302:LEU:O	1:A:306:VAL:HG23	2.06	0.55
1:A:373:ALA:HB2	1:A:397:LYS:HD3	1.89	0.55
1:D:146:LEU:O	1:D:149:ALA:HB3	2.06	0.55
1:B:250:HIS:ND1	1:B:253:THR:HG23	2.21	0.55
1:C:91:ARG:HE	4:C:600:ZDM:C57	2.18	0.55
1:D:295:MET:CE	1:D:407:ASN:HB2	2.37	0.55
1:A:240:LEU:O	1:A:244:LEU:HB2	2.06	0.55
1:B:161:ARG:HD2	1:B:162:PHE:N	2.22	0.55
1:D:246:ALA:HB1	1:D:349:LEU:HD21	1.88	0.55
1:B:176:VAL:HG23	2:E:2:NAG:C6	2.35	0.55
1:C:19:GLN:CG	1:C:22:LEU:HB2	2.35	0.55
1:D:5:LEU:O	1:D:8:TYR:HB2	2.07	0.55
1:A:205:GLU:HA	1:A:210:GLY:O	2.07	0.55
1:A:354:VAL:HG12	1:A:355:VAL:N	2.21	0.55
1:C:334:GLU:OE2	2:I:2:NAG:H61	2.06	0.55
1:C:340:MET:HB3	1:C:342:ILE:N	2.22	0.55
1:D:113:LEU:HD21	1:D:198:TRP:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:359:LEU:HD11	1:D:407:ASN:HB3	1.89	0.55
1:A:311:PHE:HD1	1:A:416:LEU:HD11	1.72	0.55
1:B:345:ASN:O	1:B:349:LEU:HB2	2.07	0.55
1:C:211:SER:HB2	1:C:213:HIS:NE2	2.21	0.55
1:D:169:ILE:HG12	1:D:185:ALA:O	2.07	0.55
1:A:301:THR:O	1:A:305:VAL:HG23	2.07	0.54
1:B:121:TYR:CD1	1:C:130:ILE:HG22	2.42	0.54
1:B:292:TRP:C	1:B:293:ILE:HD12	2.28	0.54
1:D:80:MET:CE	1:D:143:SER:HA	2.37	0.54
1:C:79:ILE:CD1	1:D:112:LEU:CD1	2.85	0.54
1:D:317:LEU:HD11	1:D:422:TRP:HD1	1.72	0.54
1:A:264:LEU:CA	1:A:267:MET:HG2	2.32	0.54
1:A:391:TYR:CE1	1:A:396:GLY:HA2	2.42	0.54
1:A:196:VAL:O	1:A:200:ILE:HG13	2.08	0.54
1:A:326:ALA:HB3	1:A:327:PRO:HD3	1.89	0.54
1:B:372:VAL:HG13	1:B:399:SER:O	2.07	0.54
1:D:299:GLY:C	1:D:301:THR:N	2.61	0.54
1:A:342:ILE:O	1:A:349:LEU:HD13	2.07	0.54
1:C:285:THR:O	1:C:288:PHE:HB3	2.08	0.54
1:D:172:MET:CG	1:D:176:VAL:HG11	2.38	0.54
1:A:320:LEU:CD2	1:A:340:MET:HB3	2.37	0.54
1:C:345:ASN:ND2	1:C:348:LEU:H	2.05	0.54
1:D:340:MET:HG2	1:D:348:LEU:CD1	2.37	0.54
1:A:4:PHE:C	1:A:6:GLU:H	2.11	0.54
1:A:191:PHE:HD1	1:B:38:ILE:HG23	1.72	0.54
1:D:189:PRO:O	1:D:193:VAL:HG23	2.08	0.54
1:D:227:LEU:O	1:D:230:SER:HB3	2.08	0.54
1:D:289:PHE:HA	1:D:293:ILE:HD13	1.90	0.54
1:D:367:MET:HB3	1:D:374:ARG:HD2	1.89	0.54
1:A:91:ARG:NE	4:A:600:ZDM:O61	2.37	0.53
1:A:119:VAL:HB	1:D:123:MET:CE	2.37	0.53
1:D:170:ILE:HG13	1:D:188:ILE:HG12	1.91	0.53
1:A:241:VAL:HG12	1:A:242:HIS:ND1	2.24	0.53
1:C:101:LEU:HD13	1:D:90:TYR:CD2	2.44	0.53
1:B:44:ILE:HD12	1:B:392:LEU:HD22	1.89	0.53
1:B:284:ILE:HG22	1:B:284:ILE:O	2.09	0.53
1:B:152:ILE:HD12	1:B:153:ALA:N	2.23	0.53
1:A:355:VAL:HG22	1:A:414:ILE:HD12	1.90	0.53
1:D:204:PHE:CD2	1:D:215:VAL:HG21	2.44	0.53
1:B:81:ALA:HB3	1:B:141:MET:O	2.09	0.53
1:C:287:GLN:NE2	1:C:379:ALA:HA	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:THR:CG2	1:D:197:VAL:HG21	2.37	0.53
1:D:319:SER:HB2	1:D:322:ARG:NH2	2.24	0.53
1:B:19:GLN:CG	1:B:22:LEU:HD13	2.39	0.53
1:D:423:ASP:O	1:D:427:ILE:HG13	2.08	0.53
1:C:381:THR:C	1:C:383:THR:N	2.62	0.53
1:D:176:VAL:HG21	1:D:180:VAL:HG11	1.91	0.53
1:A:296:GLY:HA3	1:A:302:LEU:N	2.24	0.53
1:B:289:PHE:HA	1:B:293:ILE:HD13	1.90	0.53
1:D:111:PHE:CE1	1:D:148:VAL:HG22	2.40	0.53
1:D:114:ALA:HB1	1:D:212:ILE:HD12	1.90	0.53
1:D:372:VAL:HG13	1:D:399:SER:O	2.09	0.53
1:C:355:VAL:HB	1:C:356:PRO:HD3	1.90	0.52
1:C:412:PHE:CE2	1:C:416:LEU:HD22	2.44	0.52
1:C:424:LYS:O	1:C:427:ILE:HG13	2.09	0.52
1:C:416:LEU:N	1:C:417:PRO:HD2	2.24	0.52
1:A:341:PRO:O	1:A:345:ASN:HB3	2.10	0.52
1:C:176:VAL:HG13	1:C:180:VAL:HB	1.91	0.52
1:C:367:MET:HB3	1:C:374:ARG:HD2	1.91	0.52
1:C:369:TRP:CB	1:C:371:LEU:HD12	2.39	0.52
1:D:340:MET:HB3	1:D:341:PRO:C	2.29	0.52
1:A:33:MET:SD	2:E:1:NAG:H83	2.49	0.52
1:B:301:THR:HG21	1:B:333:ASN:HB2	1.91	0.52
1:C:376:SER:HB2	1:C:378:ALA:H	1.75	0.52
1:D:22:LEU:HD21	1:D:258:VAL:CG2	2.39	0.52
4:C:600:ZDM:H10	4:C:600:ZDM:O55	2.10	0.52
1:D:106:LEU:HD21	1:D:193:VAL:HG21	1.91	0.52
1:D:296:GLY:HA2	1:D:302:LEU:HB2	1.90	0.52
1:D:410:LEU:O	1:D:414:ILE:HG13	2.10	0.52
1:C:367:MET:CE	1:C:374:ARG:HA	2.39	0.52
1:D:118:GLN:NE2	1:D:131:LEU:HD12	2.25	0.52
1:A:199:ILE:O	1:A:203:ILE:HG13	2.10	0.52
1:B:367:MET:HE2	1:B:374:ARG:HA	1.92	0.52
1:C:367:MET:HE3	1:C:374:ARG:HA	1.91	0.52
1:D:314:SER:O	1:D:318:LYS:HB2	2.10	0.52
1:B:433:GLU:O	1:B:434:ALA:HB3	2.10	0.52
1:D:89:ALA:HB1	1:D:103:SER:O	2.09	0.52
1:A:111:PHE:HE1	1:A:148:VAL:CG2	2.23	0.51
1:B:123:MET:HB3	1:B:126:THR:OG1	2.10	0.51
1:B:245:TRP:HA	1:B:249:ILE:O	2.10	0.51
1:C:398:ILE:O	1:C:398:ILE:HG22	2.10	0.51
1:D:6:GLU:OE2	1:D:9:VAL:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:VAL:HG11	1:C:213:HIS:HA	1.91	0.51
1:A:204:PHE:C	1:A:206:HIS:H	2.13	0.51
1:B:334:GLU:OE1	2:G:2:NAG:H61	2.10	0.51
1:D:124:PRO:O	1:D:126:THR:HG23	2.11	0.51
1:D:240:LEU:HB3	1:D:255:VAL:HG21	1.92	0.51
1:D:375:PRO:HA	1:D:393:GLY:O	2.10	0.51
1:C:20:ARG:HB3	1:C:95:TYR:CZ	2.46	0.51
1:D:317:LEU:HD11	1:D:422:TRP:CD1	2.45	0.51
1:D:382:TRP:HE1	2:K:1:NAG:HN2	1.58	0.51
1:D:131:LEU:HD23	1:D:131:LEU:H	1.75	0.51
1:D:287:GLN:HA	1:D:290:ASP:HB2	1.93	0.51
1:D:367:MET:HE2	1:D:374:ARG:HA	1.93	0.51
1:B:154:ILE:O	1:B:158:GLU:HB2	2.10	0.51
1:C:10:MET:N	1:C:11:PRO:CD	2.74	0.51
1:C:222:GLU:N	1:C:223:PRO:HD2	2.26	0.51
1:C:231:LEU:HD13	1:C:364:TYR:CG	2.46	0.51
1:C:297:GLY:O	2:I:2:NAG:H83	2.10	0.51
1:C:338:PHE:CE1	1:C:343:VAL:HG21	2.45	0.51
1:D:302:LEU:HG	1:D:302:LEU:O	2.10	0.51
1:A:27:ASP:CB	4:A:600:ZDM:O61	2.59	0.50
1:A:132:VAL:HG21	1:B:132:VAL:HG21	1.93	0.50
1:C:300:ALA:O	1:C:302:LEU:N	2.45	0.50
1:D:96:TYR:O	1:D:97:LYS:HB2	2.11	0.50
1:D:123:MET:HB3	1:D:126:THR:OG1	2.11	0.50
1:D:228:GLY:O	1:D:284:ILE:HG21	2.10	0.50
1:A:114:ALA:HB1	1:A:212:ILE:HD12	1.93	0.50
1:A:146:LEU:CD2	1:A:264:LEU:HD11	2.41	0.50
1:A:320:LEU:HD21	1:A:340:MET:HB3	1.94	0.50
1:B:367:MET:CE	1:B:374:ARG:HA	2.40	0.50
1:D:116:PRO:HA	1:D:201:ARG:NH2	2.27	0.50
1:A:256:GLY:C	1:A:258:VAL:H	2.15	0.50
1:A:33:MET:CB	1:A:34:PRO:HD3	2.40	0.50
1:A:46:SER:CB	1:A:69:LEU:HD12	2.41	0.50
1:B:213:HIS:HD2	1:B:214:ASN:N	2.07	0.50
1:D:25:ILE:HD13	1:D:150:MET:SD	2.52	0.50
1:A:133:ASP:HB2	1:C:128:GLU:OE2	2.12	0.50
1:B:381:THR:HG23	1:B:383:THR:H	1.76	0.50
1:C:299:GLY:C	1:C:301:THR:H	2.14	0.50
1:D:81:ALA:O	1:D:85:VAL:HG23	2.11	0.50
1:D:284:ILE:HG22	1:D:284:ILE:O	2.12	0.50
1:A:410:LEU:O	1:A:414:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:LEU:HD12	1:C:378:ALA:HB2	1.92	0.50
1:D:131:LEU:HD23	1:D:131:LEU:N	2.27	0.50
1:D:205:GLU:HA	1:D:210:GLY:O	2.11	0.50
1:B:186:ALA:O	1:B:189:PRO:HD2	2.11	0.50
1:C:43:LEU:HD13	1:C:43:LEU:O	2.12	0.50
1:D:242:HIS:HD2	1:D:356:PRO:HG2	1.77	0.50
4:A:600:ZDM:O49	1:B:182:ARG:CD	2.59	0.49
1:C:316:GLN:NE2	1:C:426:LYS:HD2	2.26	0.49
1:D:22:LEU:O	1:D:22:LEU:HD23	2.12	0.49
1:D:319:SER:O	1:D:322:ARG:HB2	2.12	0.49
1:A:367:MET:CE	1:A:375:PRO:HD3	2.30	0.49
1:C:101:LEU:HD13	1:D:90:TYR:CE2	2.46	0.49
1:C:117:PHE:CE1	1:C:136:ILE:HG12	2.47	0.49
1:C:340:MET:CB	1:C:342:ILE:HG13	2.42	0.49
5:C:444:CIT:O5	5:C:444:CIT:C1	2.60	0.49
1:D:316:GLN:OE1	1:D:426:LYS:HD2	2.12	0.49
1:B:213:HIS:CD2	1:B:213:HIS:C	2.85	0.49
1:D:44:ILE:C	1:D:44:ILE:HD12	2.32	0.49
1:A:176:VAL:HG13	1:A:180:VAL:HB	1.93	0.49
1:B:231:LEU:HD13	1:B:364:TYR:CG	2.48	0.49
1:B:336:VAL:HG13	1:B:340:MET:HG3	1.94	0.49
1:D:218:LYS:O	1:D:219:LEU:HD23	2.10	0.49
1:A:231:LEU:HD13	1:A:364:TYR:CG	2.47	0.49
1:A:310:LEU:C	1:A:311:PHE:CD2	2.85	0.49
1:C:249:ILE:HG22	1:C:250:HIS:N	2.27	0.49
1:D:80:MET:HE1	1:D:146:LEU:HD11	1.94	0.49
1:D:346:PRO:O	1:D:350:ILE:HD13	2.12	0.49
1:A:335:MET:O	1:A:339:GLY:HA3	2.11	0.49
1:B:3:ARG:O	1:B:6:GLU:HB3	2.13	0.49
1:B:252:ALA:HB2	2:G:2:NAG:O7	2.13	0.49
1:C:325:ILE:HG23	1:C:326:ALA:H	1.77	0.49
4:C:443:ZDM:C57	1:D:91:ARG:HE	2.25	0.49
1:D:359:LEU:HD13	1:D:407:ASN:HB3	1.95	0.49
1:B:86:PHE:CD1	1:B:104:GLY:O	2.66	0.49
1:C:269:GLN:HE21	1:C:282:ASN:ND2	2.08	0.49
1:D:216:VAL:HG13	1:D:220:LEU:HD12	1.94	0.49
1:A:10:MET:N	1:A:11:PRO:CD	2.75	0.49
1:B:10:MET:N	1:B:11:PRO:HD2	2.27	0.49
1:B:145:GLY:O	1:B:148:VAL:HG12	2.13	0.49
1:C:386:ILE:O	1:C:389:SER:HB3	2.13	0.49
1:D:225:SER:HA	1:D:262:ILE:HG23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:VAL:HG21	1:B:38:ILE:HG21	1.94	0.49
1:A:326:ALA:HB3	1:A:327:PRO:CD	2.42	0.49
1:A:386:ILE:HG23	1:A:387:LEU:N	2.27	0.49
1:C:165:GLN:C	1:C:167:LYS:H	2.15	0.49
1:A:415:TYR:C	1:A:417:PRO:HD2	2.33	0.48
1:D:176:VAL:HG23	2:I:2:NAG:C6	2.43	0.48
1:B:242:HIS:HD2	1:B:356:PRO:HG2	1.76	0.48
1:C:293:ILE:HG12	1:C:360:THR:OG1	2.12	0.48
1:C:340:MET:CG	1:C:342:ILE:HG13	2.43	0.48
1:B:287:GLN:HB3	1:B:291:LEU:CD1	2.44	0.48
1:D:426:LYS:O	1:D:430:GLU:HG3	2.13	0.48
3:J:1:GLC:O3	3:J:2:GLC:O5	2.18	0.48
1:A:345:ASN:HD21	1:A:348:LEU:N	2.10	0.48
1:B:310:LEU:HB3	1:B:311:PHE:CD2	2.48	0.48
1:A:242:HIS:NE2	1:A:298:SER:O	2.47	0.48
1:C:408:PHE:O	1:C:408:PHE:CD1	2.66	0.48
1:D:43:LEU:CD1	1:D:378:ALA:HB2	2.41	0.48
1:D:117:PHE:HA	1:D:135:VAL:O	2.14	0.48
1:D:242:HIS:NE2	1:D:298:SER:O	2.46	0.48
1:A:10:MET:N	1:A:11:PRO:HD2	2.29	0.48
1:A:256:GLY:O	1:A:258:VAL:N	2.47	0.48
1:C:367:MET:CE	1:C:375:PRO:HD3	2.37	0.48
1:D:74:SER:O	1:D:78:ASN:HB2	2.13	0.48
1:D:264:LEU:HA	1:D:267:MET:CB	2.44	0.48
1:B:48:LEU:HB3	1:B:53:TYR:CE2	2.48	0.48
1:D:112:LEU:O	1:D:117:PHE:HE2	1.97	0.48
1:D:184:PHE:H	1:D:184:PHE:HD2	1.61	0.48
1:D:287:GLN:CD	1:D:287:GLN:N	2.64	0.48
1:A:227:LEU:O	1:A:230:SER:HB3	2.13	0.48
1:A:386:ILE:HG23	1:A:387:LEU:HG	1.96	0.48
1:C:368:GLU:C	1:C:370:GLY:H	2.16	0.48
1:A:222:GLU:N	1:A:223:PRO:HD2	2.29	0.47
1:C:240:LEU:HA	1:C:243:VAL:HG22	1.95	0.47
1:C:316:GLN:NE2	1:C:426:LYS:HB3	2.29	0.47
1:D:48:LEU:HA	1:D:49:PRO:HD3	1.62	0.47
1:A:298:SER:HB3	1:A:352:PHE:CZ	2.49	0.47
1:A:368:GLU:C	1:A:370:GLY:H	2.18	0.47
1:B:366:ALA:HB1	1:B:372:VAL:CG2	2.44	0.47
1:A:79:ILE:O	1:A:79:ILE:CG2	2.62	0.47
1:B:242:HIS:NE2	1:B:298:SER:O	2.47	0.47
1:C:231:LEU:HD13	1:C:364:TYR:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:VAL:HA	1:C:399:SER:HB2	1.96	0.47
1:D:268:ASP:OD1	1:D:271:ARG:NH1	2.44	0.47
1:A:38:ILE:CG2	1:B:194:VAL:HG21	2.44	0.47
1:A:311:PHE:CD1	1:A:416:LEU:HD11	2.50	0.47
1:B:163:LEU:HD11	1:B:192:ILE:HG21	1.96	0.47
1:B:325:ILE:HD12	1:B:326:ALA:H	1.79	0.47
1:D:269:GLN:H	1:D:269:GLN:HG2	1.56	0.47
1:D:336:VAL:HG12	1:D:342:ILE:CD1	2.44	0.47
1:A:163:LEU:HD13	1:A:189:PRO:HA	1.96	0.47
1:B:79:ILE:O	1:B:80:MET:C	2.52	0.47
1:B:204:PHE:CE1	1:B:215:VAL:HG11	2.49	0.47
1:C:176:VAL:O	1:C:176:VAL:HG12	2.15	0.47
1:C:274:PHE:HB2	1:C:280:VAL:CG1	2.45	0.47
1:C:386:ILE:HG23	1:C:387:LEU:N	2.29	0.47
1:A:80:MET:HE2	1:A:143:SER:CA	2.43	0.47
1:A:171:LYS:O	1:A:171:LYS:HG3	2.14	0.47
1:A:241:VAL:HG23	1:A:255:VAL:HG21	1.96	0.47
1:B:106:LEU:HD21	1:B:193:VAL:HG11	1.95	0.47
1:C:295:MET:HG2	1:C:386:ILE:HG13	1.96	0.47
1:D:204:PHE:HA	1:D:207:THR:CG2	2.44	0.47
1:D:295:MET:SD	1:D:386:ILE:HD11	2.55	0.47
1:A:83:ILE:HD11	1:B:109:VAL:CG2	2.44	0.47
1:C:110:THR:HG22	1:C:152:ILE:HD13	1.97	0.47
1:C:176:VAL:HG22	2:K:2:NAG:H62	1.97	0.47
1:C:293:ILE:HG22	1:C:294:TYR:CD1	2.50	0.47
1:D:253:THR:HG22	2:K:1:NAG:H1	1.97	0.47
1:A:312:ALA:HB1	1:A:318:LYS:HB2	1.97	0.47
1:B:50:ILE:HA	1:B:51:PRO:HD3	1.78	0.47
1:C:245:TRP:HA	1:C:249:ILE:O	2.15	0.47
1:C:259:MET:C	1:C:261:PRO:HD2	2.34	0.47
1:D:68:ALA:HA	1:D:71:TYR:CE2	2.49	0.47
1:A:182:ARG:O	1:A:185:ALA:HB3	2.15	0.47
1:B:110:THR:HG23	1:B:197:VAL:HG21	1.96	0.47
1:C:46:SER:HB2	1:C:69:LEU:HB3	1.95	0.47
1:C:79:ILE:HD11	1:D:112:LEU:HD12	1.96	0.47
1:C:292:TRP:HA	1:C:295:MET:HE3	1.97	0.47
1:D:91:ARG:HD2	1:D:91:ARG:O	2.15	0.47
1:D:345:ASN:ND2	1:D:348:LEU:HB2	2.30	0.47
1:B:193:VAL:O	1:B:197:VAL:HG23	2.16	0.46
1:B:226:ILE:HD12	1:B:226:ILE:HA	1.73	0.46
1:C:20:ARG:HD3	1:C:95:TYR:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:PRO:HB2	1:D:415:TYR:CE1	2.50	0.46
1:D:398:ILE:HG22	1:D:398:ILE:O	2.14	0.46
1:B:287:GLN:HB3	1:B:291:LEU:HD11	1.97	0.46
1:C:295:MET:HE2	1:C:404:GLN:HG2	1.98	0.46
1:D:264:LEU:HA	1:D:267:MET:HB3	1.97	0.46
1:C:267:MET:HB3	1:C:267:MET:HE2	1.77	0.46
1:A:86:PHE:CZ	1:B:86:PHE:CZ	3.04	0.46
1:A:296:GLY:CA	1:A:302:LEU:HB2	2.44	0.46
1:A:398:ILE:N	1:A:398:ILE:HD12	2.31	0.46
1:B:148:VAL:O	1:B:152:ILE:HG13	2.16	0.46
1:B:310:LEU:HB3	1:B:311:PHE:HD2	1.79	0.46
1:C:291:LEU:HD22	1:C:389:SER:OG	2.15	0.46
1:C:298:SER:HB3	1:C:352:PHE:HZ	1.80	0.46
1:D:9:VAL:HG22	1:D:247:CYS:SG	2.56	0.46
1:D:340:MET:N	1:D:341:PRO:HA	2.29	0.46
1:A:298:SER:N	1:A:333:ASN:ND2	2.57	0.46
1:B:40:SER:O	1:B:44:ILE:HG23	2.16	0.46
1:B:10:MET:N	1:B:11:PRO:CD	2.79	0.46
1:B:303:ALA:HA	1:B:408:PHE:HE1	1.80	0.46
1:C:326:ALA:N	1:C:327:PRO:HD2	2.31	0.46
1:C:383:THR:O	1:C:383:THR:HG22	2.14	0.46
1:D:145:GLY:O	1:D:148:VAL:HG13	2.15	0.46
3:L:1:GLC:O3	3:L:2:GLC:O5	2.31	0.46
1:A:146:LEU:HD12	1:A:147:PHE:N	2.31	0.46
1:A:357:VAL:O	1:A:361:ILE:HG13	2.15	0.46
1:B:111:PHE:HE1	1:B:148:VAL:HG13	1.81	0.46
1:C:146:LEU:HA	1:C:149:ALA:CB	2.46	0.46
1:C:220:LEU:HD23	1:C:220:LEU:HA	1.72	0.46
1:C:325:ILE:HG23	1:C:326:ALA:N	2.31	0.46
1:D:80:MET:CE	1:D:146:LEU:HD11	2.46	0.46
1:D:110:THR:HG23	1:D:197:VAL:HG11	1.97	0.46
1:A:402:ILE:HG13	1:A:403:LEU:N	2.30	0.46
1:C:146:LEU:HA	1:C:149:ALA:HB2	1.98	0.46
1:C:222:GLU:O	1:C:226:ILE:HG12	2.16	0.46
1:A:262:ILE:O	1:A:266:LEU:HG	2.15	0.46
1:C:118:GLN:HE21	1:C:131:LEU:HD11	1.81	0.46
1:C:264:LEU:HA	1:C:267:MET:HB3	1.97	0.46
1:C:37:ILE:HG21	1:D:187:LEU:HD21	1.98	0.45
1:D:100:ALA:O	1:D:101:LEU:C	2.54	0.45
1:B:7:LYS:C	1:B:8:TYR:CD2	2.90	0.45
1:C:6:GLU:OE2	1:C:9:VAL:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:HIS:CD2	1:C:298:SER:O	2.70	0.45
1:D:354:VAL:HG12	1:D:355:VAL:N	2.31	0.45
1:A:291:LEU:HD11	1:A:380:VAL:CG1	2.47	0.45
1:C:121:TYR:HB2	1:C:130:ILE:HG23	1.98	0.45
1:D:270:ASN:OD1	1:D:282:ASN:OD1	2.34	0.45
1:A:204:PHE:HE1	1:A:215:VAL:HG21	1.80	0.45
1:B:316:GLN:HB2	1:B:430:GLU:OE2	2.16	0.45
1:B:410:LEU:O	1:B:413:VAL:HG22	2.16	0.45
1:B:394:SER:HB3	1:B:397:LYS:HB2	1.97	0.45
1:C:71:TYR:HB2	1:C:72:PRO:CD	2.45	0.45
1:C:398:ILE:O	1:C:398:ILE:CG2	2.65	0.45
1:D:200:ILE:HG22	1:D:212:ILE:HD11	1.97	0.45
1:D:367:MET:HE3	1:D:375:PRO:HD3	1.98	0.45
1:D:391:TYR:HB2	1:D:401:VAL:CG2	2.47	0.45
1:B:365:PHE:O	1:B:366:ALA:C	2.55	0.45
1:C:85:VAL:HG12	1:C:149:ALA:HA	1.98	0.45
1:A:121:TYR:CE1	1:D:123:MET:HB2	2.52	0.45
1:A:290:ASP:OD2	1:A:382:TRP:HB3	2.16	0.45
1:B:170:ILE:HB	1:B:184:PHE:O	2.16	0.45
1:D:43:LEU:HD12	1:D:378:ALA:CB	2.47	0.45
1:D:325:ILE:HG13	1:D:326:ALA:H	1.82	0.45
1:A:161:ARG:HD2	1:A:162:PHE:N	2.32	0.45
1:B:36:LEU:HD21	1:B:80:MET:CG	2.45	0.45
1:B:340:MET:HB2	1:B:341:PRO:C	2.37	0.45
1:D:6:GLU:OE2	1:D:6:GLU:HA	2.17	0.45
1:A:386:ILE:O	1:A:404:GLN:NE2	2.50	0.45
1:B:152:ILE:HD12	1:B:152:ILE:C	2.37	0.45
1:B:253:THR:HG22	2:G:1:NAG:H1	1.98	0.45
1:C:407:ASN:C	1:C:409:ALA:H	2.19	0.45
3:F:1:GLC:H62	3:F:2:GLC:O2	2.17	0.45
1:A:96:TYR:CD2	1:A:161:ARG:CG	2.94	0.45
1:A:284:ILE:HD11	1:A:364:TYR:CD1	2.51	0.45
1:B:308:MET:HB2	1:B:308:MET:HE2	1.91	0.45
1:B:146:LEU:HA	1:B:149:ALA:CB	2.47	0.44
1:B:146:LEU:HD21	1:B:264:LEU:HD13	1.99	0.44
1:C:20:ARG:HG3	1:C:21:HIS:H	1.81	0.44
1:C:110:THR:HG21	1:C:197:VAL:HG21	2.00	0.44
1:C:146:LEU:HD21	1:C:264:LEU:CD1	2.46	0.44
1:C:213:HIS:CD2	1:C:214:ASN:H	2.21	0.44
1:C:368:GLU:C	1:C:370:GLY:N	2.71	0.44
1:A:115:THR:HA	1:A:116:PRO:HD3	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:TRP:CE3	1:B:383:THR:HG22	2.52	0.44
1:C:260:SER:HA	1:C:263:TRP:HB2	2.00	0.44
1:C:298:SER:N	1:C:333:ASN:ND2	2.60	0.44
1:D:80:MET:HE2	1:D:80:MET:HB2	1.55	0.44
1:D:182:ARG:O	1:D:185:ALA:HB3	2.18	0.44
1:D:203:ILE:O	1:D:207:THR:HG23	2.17	0.44
1:B:226:ILE:HG22	1:B:227:LEU:N	2.31	0.44
1:B:260:SER:N	1:B:261:PRO:CD	2.80	0.44
1:C:72:PRO:HD3	1:D:198:TRP:CD1	2.52	0.44
1:D:410:LEU:O	1:D:413:VAL:HG22	2.16	0.44
1:B:372:VAL:HG11	1:B:403:LEU:HD22	1.99	0.44
1:C:48:LEU:HA	1:C:49:PRO:HD3	1.77	0.44
1:C:206:HIS:O	1:C:207:THR:HG23	2.17	0.44
1:C:340:MET:HB3	1:C:341:PRO:C	2.37	0.44
1:D:348:LEU:HA	1:D:348:LEU:HD23	1.74	0.44
1:A:119:VAL:HB	1:D:123:MET:HE3	1.99	0.44
1:A:284:ILE:HD11	1:A:364:TYR:HD1	1.83	0.44
1:B:376:SER:HB3	1:B:395:GLY:HA3	1.99	0.44
1:C:91:ARG:C	1:C:93:GLY:N	2.70	0.44
1:C:290:ASP:OD2	1:C:382:TRP:HB3	2.17	0.44
1:D:309:LEU:O	1:D:310:LEU:HD23	2.17	0.44
1:A:36:LEU:HD23	1:A:36:LEU:N	2.32	0.44
1:B:85:VAL:HG21	1:B:152:ILE:HD11	1.99	0.44
1:B:331:ASN:N	1:B:331:ASN:ND2	2.65	0.44
1:C:169:ILE:HG23	1:C:185:ALA:HA	1.99	0.44
1:A:81:ALA:HB2	1:A:146:LEU:N	2.32	0.44
1:A:96:TYR:CE2	1:A:161:ARG:NE	2.85	0.44
1:A:382:TRP:CH2	1:A:383:THR:HG22	2.52	0.44
1:B:306:VAL:O	1:B:310:LEU:HB2	2.17	0.44
1:B:367:MET:HA	1:B:372:VAL:O	2.18	0.44
1:C:173:PRO:O	1:C:176:VAL:HB	2.17	0.44
1:D:131:LEU:N	1:D:131:LEU:CD2	2.80	0.44
1:D:252:ALA:HB2	2:K:2:NAG:O7	2.17	0.44
1:A:176:VAL:HG22	2:G:2:NAG:H62	1.99	0.44
1:B:368:GLU:C	1:B:370:GLY:N	2.70	0.44
1:D:382:TRP:CE3	1:D:383:THR:HG22	2.52	0.44
1:A:25:ILE:HA	1:A:88:ILE:HG12	1.98	0.44
1:A:96:TYR:CE2	1:A:161:ARG:HG2	2.52	0.44
1:A:293:ILE:O	1:A:295:MET:N	2.50	0.44
1:A:314:SER:HB3	1:A:423:ASP:OD2	2.18	0.44
1:C:46:SER:HB2	1:C:69:LEU:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:VAL:O	1:C:242:HIS:ND1	2.51	0.44
1:D:268:ASP:O	1:D:269:GLN:C	2.55	0.44
1:A:79:ILE:HG23	1:A:82:LEU:HB3	2.00	0.43
1:A:165:GLN:C	1:A:167:LYS:H	2.22	0.43
1:A:215:VAL:HG13	1:A:216:VAL:N	2.33	0.43
1:A:222:GLU:H	1:A:223:PRO:HD2	1.83	0.43
1:A:352:PHE:HA	1:A:415:TYR:OH	2.17	0.43
1:A:361:ILE:C	1:A:363:SER:H	2.21	0.43
1:C:110:THR:CG2	1:C:197:VAL:HG21	2.48	0.43
1:A:330:PHE:O	1:A:331:ASN:HB2	2.18	0.43
1:B:48:LEU:O	1:B:53:TYR:HD2	2.01	0.43
1:B:207:THR:OG1	1:B:209:PHE:HD2	2.01	0.43
1:B:274:PHE:C	1:B:276:ALA:H	2.22	0.43
1:B:278:GLN:HG2	1:B:279:ASP:H	1.82	0.43
1:B:349:LEU:HD12	1:B:349:LEU:HA	1.78	0.43
1:B:10:MET:SD	1:B:247:CYS:HB3	2.58	0.43
1:B:118:GLN:HA	1:B:135:VAL:HG12	2.01	0.43
1:B:229:ALA:HB2	1:B:266:LEU:CD1	2.48	0.43
1:C:147:PHE:HA	1:C:150:MET:CE	2.47	0.43
1:C:391:TYR:CE1	1:C:396:GLY:O	2.72	0.43
1:B:386:ILE:HG23	1:B:387:LEU:HG	2.00	0.43
1:C:375:PRO:O	1:C:376:SER:C	2.57	0.43
1:D:32:THR:HG22	1:D:83:ILE:HB	2.01	0.43
1:D:56:PHE:CE2	1:D:60:LEU:HD11	2.53	0.43
1:D:85:VAL:HG12	1:D:107:SER:HB3	1.99	0.43
1:C:113:LEU:HD21	1:C:198:TRP:HB2	2.00	0.43
1:C:431:LYS:HE2	1:C:433:GLU:CD	2.39	0.43
1:A:9:VAL:C	1:A:11:PRO:HD2	2.39	0.43
1:A:246:ALA:CB	1:A:349:LEU:HD21	2.45	0.43
1:A:310:LEU:HB3	1:A:311:PHE:CE2	2.54	0.43
1:A:387:LEU:HA	1:A:404:GLN:NE2	2.26	0.43
1:C:79:ILE:HG12	1:C:82:LEU:HB3	2.01	0.43
1:D:146:LEU:O	1:D:150:MET:HG3	2.18	0.43
1:D:260:SER:HA	1:D:263:TRP:HB2	1.99	0.43
1:A:146:LEU:HA	1:A:149:ALA:CB	2.49	0.43
1:A:349:LEU:HD12	1:A:349:LEU:HA	1.90	0.43
1:C:336:VAL:O	1:C:340:MET:HB2	2.18	0.43
1:D:291:LEU:HB3	1:D:389:SER:OG	2.18	0.43
1:A:219:LEU:N	1:A:219:LEU:HD23	2.34	0.43
1:C:79:ILE:HA	1:C:141:MET:O	2.18	0.43
1:D:65:TRP:CG	1:D:66:ASN:N	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:ALA:HB3	1:D:141:MET:O	2.18	0.43
1:D:232:TRP:O	1:D:236:ILE:HG13	2.19	0.43
1:D:305:VAL:HA	1:D:308:MET:HE2	2.01	0.43
1:C:43:LEU:HD13	1:C:43:LEU:C	2.39	0.43
1:C:80:MET:HE1	1:C:264:LEU:HD13	2.00	0.43
1:C:369:TRP:HB3	1:C:371:LEU:CD1	2.49	0.43
1:B:3:ARG:HG3	1:B:344:MET:HG3	2.00	0.43
1:B:280:VAL:HA	1:B:281:PRO:HD2	1.86	0.43
1:B:387:LEU:HD22	1:B:401:VAL:HG13	1.99	0.43
1:C:199:ILE:O	1:C:203:ILE:HG13	2.18	0.43
1:D:82:LEU:HD12	1:D:82:LEU:HA	1.69	0.43
1:B:320:LEU:CD2	1:B:340:MET:HG2	2.49	0.42
1:B:354:VAL:O	1:B:357:VAL:HG22	2.19	0.42
1:D:79:ILE:O	1:D:80:MET:C	2.56	0.42
1:D:184:PHE:N	1:D:184:PHE:CD2	2.87	0.42
1:A:79:ILE:HG23	1:A:79:ILE:HD12	1.77	0.42
1:A:151:ILE:O	1:A:155:ILE:HB	2.19	0.42
1:A:217:GLY:HA2	1:A:221:GLN:HB3	2.01	0.42
1:A:317:LEU:HD11	1:A:422:TRP:CD1	2.51	0.42
1:B:229:ALA:HB2	1:B:266:LEU:HD13	2.02	0.42
1:B:241:VAL:HG12	1:B:242:HIS:ND1	2.34	0.42
1:B:325:ILE:H	1:B:325:ILE:HG13	1.70	0.42
1:C:204:PHE:HE1	1:C:215:VAL:HG11	1.83	0.42
1:C:416:LEU:HD12	1:C:416:LEU:HA	1.69	0.42
1:D:171:LYS:O	1:D:171:LYS:HG3	2.20	0.42
1:D:316:GLN:O	1:D:319:SER:HB3	2.19	0.42
1:A:43:LEU:O	1:A:47:THR:HG23	2.18	0.42
1:A:146:LEU:HA	1:A:149:ALA:HB3	2.00	0.42
1:B:48:LEU:HA	1:B:49:PRO:HD3	1.72	0.42
1:B:116:PRO:HB3	1:B:201:ARG:HH21	1.85	0.42
1:C:304:LEU:O	1:C:308:MET:HG3	2.18	0.42
1:D:426:LYS:HA	1:D:426:LYS:HD3	1.87	0.42
1:B:166:LYS:HA	1:B:166:LYS:HD3	1.50	0.42
1:C:292:TRP:CD1	1:C:403:LEU:HD23	2.55	0.42
1:A:283:THR:HA	1:A:374:ARG:HG3	2.02	0.42
1:A:308:MET:HG2	1:A:419:LEU:HD11	2.02	0.42
1:C:369:TRP:CZ3	3:J:1:GLC:H2	2.55	0.42
1:D:98:VAL:HG11	1:D:161:ARG:HA	2.02	0.42
1:D:240:LEU:HD23	1:D:240:LEU:HA	1.67	0.42
1:A:381:THR:HG23	1:A:383:THR:H	1.85	0.42
1:C:48:LEU:HA	1:C:48:LEU:HD23	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:VAL:HG23	2:I:2:NAG:H62	2.02	0.42
1:D:325:ILE:O	1:D:328:GLY:N	2.52	0.42
1:B:71:TYR:CB	1:B:72:PRO:HD3	2.48	0.42
1:B:110:THR:HG21	1:B:156:SER:OG	2.19	0.42
1:B:293:ILE:HD12	1:B:293:ILE:N	2.34	0.42
1:C:36:LEU:HD21	1:C:80:MET:HG2	2.02	0.42
1:C:383:THR:O	1:C:383:THR:CG2	2.68	0.42
1:A:158:GLU:O	1:A:161:ARG:HG3	2.18	0.42
1:A:272:ILE:HG22	1:A:273:ALA:N	2.34	0.42
1:A:312:ALA:HB1	1:A:318:LYS:CB	2.49	0.42
1:B:300:ALA:HB3	1:B:411:ALA:HB1	2.01	0.42
1:A:163:LEU:CD1	1:A:189:PRO:HA	2.50	0.42
1:C:46:SER:HB2	1:C:69:LEU:HD12	2.02	0.42
1:C:221:GLN:O	1:C:225:SER:HB2	2.19	0.42
1:A:205:GLU:HG2	1:A:210:GLY:O	2.20	0.42
1:A:287:GLN:NE2	1:A:287:GLN:H	2.18	0.42
1:B:218:LYS:HD3	1:B:218:LYS:HA	1.90	0.42
1:B:329:ILE:HG22	1:B:330:PHE:CD1	2.55	0.42
1:C:68:ALA:C	1:C:70:GLY:H	2.22	0.42
1:C:92:LEU:HD23	1:C:157:THR:HB	2.02	0.42
1:D:79:ILE:O	1:D:79:ILE:HG22	2.20	0.42
1:D:119:VAL:HG13	1:D:137:PRO:HB3	2.01	0.42
1:D:242:HIS:ND1	1:D:242:HIS:N	2.65	0.42
1:D:315:GLN:OE1	1:D:315:GLN:HA	2.19	0.42
1:B:176:VAL:CG2	1:B:177:PRO:HD2	2.50	0.41
1:B:176:VAL:O	1:B:176:VAL:HG13	2.20	0.41
1:C:298:SER:HB3	1:C:352:PHE:CE1	2.55	0.41
1:D:34:PRO:O	1:D:38:ILE:HG13	2.19	0.41
1:D:386:ILE:CG2	1:D:387:LEU:N	2.83	0.41
1:A:110:THR:HG22	1:A:152:ILE:HG23	2.02	0.41
1:A:398:ILE:C	1:A:400:GLY:H	2.24	0.41
1:B:240:LEU:HD23	1:B:240:LEU:HA	1.86	0.41
1:B:283:THR:HG23	1:B:367:MET:SD	2.60	0.41
1:B:416:LEU:HD12	1:B:416:LEU:HA	1.84	0.41
1:D:85:VAL:HG13	1:D:153:ALA:HB2	2.01	0.41
1:D:365:PHE:O	1:D:367:MET:N	2.53	0.41
1:D:375:PRO:C	1:D:377:GLY:H	2.24	0.41
1:A:4:PHE:C	1:A:6:GLU:N	2.73	0.41
1:A:182:ARG:HD3	4:A:443:ZDM:O49	2.18	0.41
1:A:231:LEU:HD13	1:A:364:TYR:CD2	2.55	0.41
1:A:358:VAL:HG12	1:A:359:LEU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:LEU:HD11	1:B:380:VAL:CG1	2.50	0.41
1:A:296:GLY:HA2	1:A:302:LEU:HB2	2.02	0.41
1:B:50:ILE:HB	1:B:53:TYR:HB2	2.01	0.41
1:B:107:SER:HA	1:B:110:THR:HB	2.02	0.41
1:B:278:GLN:HG2	1:B:279:ASP:N	2.35	0.41
1:B:287:GLN:H	1:B:287:GLN:CD	2.24	0.41
1:D:20:ARG:HB3	1:D:95:TYR:CZ	2.56	0.41
1:A:344:MET:O	1:A:344:MET:HG3	2.20	0.41
1:C:205:GLU:HA	1:C:210:GLY:O	2.21	0.41
1:C:336:VAL:O	1:C:337:THR:C	2.59	0.41
1:D:92:LEU:HD23	1:D:157:THR:HB	2.02	0.41
1:A:24:ALA:HB1	1:A:92:LEU:HB2	2.01	0.41
1:A:242:HIS:CD2	1:A:356:PRO:HG2	2.55	0.41
1:A:369:TRP:CB	1:A:371:LEU:HD12	2.49	0.41
1:B:10:MET:CG	1:B:247:CYS:HB3	2.48	0.41
1:C:117:PHE:CE1	1:C:136:ILE:CG1	3.02	0.41
1:C:184:PHE:H	1:C:184:PHE:HD2	1.67	0.41
1:A:369:TRP:CZ3	3:F:1:GLC:H2	2.55	0.41
1:D:80:MET:HE1	1:D:143:SER:HA	2.02	0.41
1:D:309:LEU:CD1	1:D:325:ILE:HG21	2.51	0.41
1:A:412:PHE:O	1:A:416:LEU:HB2	2.20	0.41
1:B:43:LEU:HD12	1:B:378:ALA:HB2	2.02	0.41
1:D:112:LEU:HD23	1:D:112:LEU:HA	1.73	0.41
1:D:217:GLY:HA2	1:D:221:GLN:HB3	2.02	0.41
1:A:24:ALA:CB	1:A:92:LEU:HB2	2.51	0.41
1:A:71:TYR:CB	1:A:72:PRO:HD3	2.50	0.41
1:A:308:MET:HE3	1:A:321:GLY:N	2.36	0.41
1:B:204:PHE:HA	1:B:207:THR:CG2	2.48	0.41
1:B:308:MET:HA	1:B:312:ALA:HB2	2.03	0.41
1:B:369:TRP:N	1:B:369:TRP:CE3	2.89	0.41
1:B:387:LEU:HD23	1:B:387:LEU:HA	1.83	0.41
1:C:37:ILE:HG12	1:C:381:THR:HG23	2.03	0.41
1:C:340:MET:HB3	1:C:342:ILE:HG13	2.02	0.41
1:C:382:TRP:HE1	2:I:1:NAG:HN2	1.69	0.41
1:C:355:VAL:O	1:C:359:LEU:HB2	2.21	0.41
1:D:119:VAL:O	1:D:132:VAL:HG22	2.21	0.41
1:D:376:SER:HB3	1:D:395:GLY:CA	2.51	0.41
1:A:32:THR:HG21	1:A:84:ALA:HB2	2.01	0.40
1:A:117:PHE:HA	1:A:135:VAL:O	2.20	0.40
1:B:91:ARG:C	1:B:93:GLY:N	2.73	0.40
1:B:335:MET:HA	1:B:335:MET:HE3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:PHE:C	1:C:6:GLU:H	2.25	0.40
1:C:300:ALA:HB3	1:C:355:VAL:HG11	2.03	0.40
1:A:120:ALA:O	1:D:123:MET:HG3	2.21	0.40
1:A:162:PHE:CE2	1:A:166:LYS:HD2	2.56	0.40
1:C:136:ILE:HA	1:C:137:PRO:HD3	1.90	0.40
1:C:417:PRO:HG2	1:C:418:PHE:CD2	2.56	0.40
1:D:122:ILE:HD12	1:D:122:ILE:HA	1.91	0.40
1:C:353:ILE:HG22	1:C:353:ILE:O	2.21	0.40
1:D:254:ILE:N	1:D:254:ILE:HD13	2.34	0.40
1:D:365:PHE:O	1:D:366:ALA:C	2.59	0.40
1:A:90:TYR:CE2	1:B:101:LEU:HD13	2.55	0.40
1:A:110:THR:HG23	1:A:197:VAL:HG21	2.03	0.40
1:A:331:ASN:HD22	1:A:331:ASN:N	2.19	0.40
1:C:75:ALA:O	1:C:79:ILE:HG21	2.21	0.40
1:C:295:MET:HG2	1:C:386:ILE:HD11	2.03	0.40
1:C:316:GLN:HE21	1:C:426:LYS:HB3	1.85	0.40
1:D:30:VAL:HA	1:D:33:MET:HG3	2.03	0.40
1:A:260:SER:HA	1:A:263:TRP:HB2	2.03	0.40
1:A:433:GLU:HG2	1:A:434:ALA:H	1.87	0.40
1:B:41:ILE:O	1:B:45:ILE:HB	2.21	0.40
1:B:186:ALA:O	1:B:187:LEU:C	2.60	0.40
1:B:242:HIS:CD2	1:B:298:SER:O	2.75	0.40
1:D:79:ILE:O	1:D:82:LEU:N	2.52	0.40
1:D:85:VAL:CG2	1:D:149:ALA:HB1	2.51	0.40
1:D:234:ALA:HB2	1:D:284:ILE:CG1	2.52	0.40
1:D:366:ALA:HB1	1:D:372:VAL:CG2	2.51	0.40
1:D:387:LEU:HD21	1:D:405:LEU:HD21	2.03	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	430/442 (97%)	339 (79%)	84 (20%)	7 (2%)	9	36
1	B	430/442 (97%)	365 (85%)	60 (14%)	5 (1%)	13	42
1	C	430/442 (97%)	355 (83%)	67 (16%)	8 (2%)	8	34
1	D	434/442 (98%)	353 (81%)	70 (16%)	11 (2%)	5	27
All	All	1724/1768 (98%)	1412 (82%)	281 (16%)	31 (2%)	8	35

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	341	PRO
1	C	301	THR
1	D	301	THR
1	B	301	THR
1	B	369	TRP
1	A	257	GLY
1	B	150	MET
1	B	177	PRO
1	A	294	TYR
1	C	273	ALA
1	D	177	PRO
1	D	366	ALA
1	A	369	TRP
1	C	5	LEU
1	D	183	SER
1	D	261	PRO
1	D	294	TYR
1	D	386	ILE
1	A	362	VAL
1	C	366	ALA
1	C	369	TRP
1	D	423	ASP
1	D	116	PRO
1	D	137	PRO
1	D	281	PRO
1	B	297	GLY
1	A	256	GLY
1	A	340	MET
1	C	173	PRO
1	C	79	ILE
1	C	297	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	345/361 (96%)	325 (94%)	20 (6%)	20	50
1	B	348/361 (96%)	324 (93%)	24 (7%)	15	44
1	C	346/361 (96%)	327 (94%)	19 (6%)	21	52
1	D	349/361 (97%)	314 (90%)	35 (10%)	7	27
All	All	1388/1444 (96%)	1290 (93%)	98 (7%)	14	42

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ARG
1	A	23	LEU
1	A	46	SER
1	A	108	LEU
1	A	146	LEU
1	A	147	PHE
1	A	176	VAL
1	A	213	HIS
1	A	240	LEU
1	A	244	LEU
1	A	267	MET
1	A	272	ILE
1	A	287	GLN
1	A	301	THR
1	A	345	ASN
1	A	354	VAL
1	A	369	TRP
1	A	374	ARG
1	A	410	LEU
1	A	415	TYR
1	B	3	ARG
1	B	4	PHE
1	B	6	GLU
1	B	79	ILE

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Mol	Chain	Res	Type
1	B	118	GLN
1	B	135	VAL
1	B	146	LEU
1	B	147	PHE
1	B	171	LYS
1	B	209	PHE
1	B	213	HIS
1	B	226	ILE
1	B	242	HIS
1	B	264	LEU
1	B	271	ARG
1	B	280	VAL
1	B	301	THR
1	B	329	ILE
1	B	331	ASN
1	B	335	MET
1	B	369	TRP
1	B	374	ARG
1	B	389	SER
1	B	419	LEU
1	C	19	GLN
1	C	23	LEU
1	C	135	VAL
1	C	144	GLN
1	C	146	LEU
1	C	147	PHE
1	C	161	ARG
1	C	205	GLU
1	C	213	HIS
1	C	225	SER
1	C	240	LEU
1	C	264	LEU
1	C	267	MET
1	C	329	ILE
1	C	331	ASN
1	C	354	VAL
1	C	369	TRP
1	C	374	ARG
1	C	415	TYR
1	D	9	VAL
1	D	20	ARG
1	D	44	ILE

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Mol	Chain	Res	Type
1	D	66	ASN
1	D	91	ARG
1	D	108	LEU
1	D	116	PRO
1	D	130	ILE
1	D	131	LEU
1	D	135	VAL
1	D	148	VAL
1	D	156	SER
1	D	168	MET
1	D	169	ILE
1	D	193	VAL
1	D	205	GLU
1	D	211	SER
1	D	235	VAL
1	D	242	HIS
1	D	269	GLN
1	D	271	ARG
1	D	280	VAL
1	D	284	ILE
1	D	287	GLN
1	D	309	LEU
1	D	329	ILE
1	D	340	MET
1	D	359	LEU
1	D	369	TRP
1	D	374	ARG
1	D	388	PHE
1	D	389	SER
1	D	408	PHE
1	D	415	TYR
1	D	425	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	A	206	HIS
1	A	287	GLN
1	A	316	GLN
1	A	331	ASN
1	A	333	ASN

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Mol	Chain	Res	Type
1	A	345	ASN
1	A	404	GLN
1	B	213	HIS
1	B	221	GLN
1	B	316	GLN
1	B	331	ASN
1	C	118	GLN
1	C	213	HIS
1	C	282	ASN
1	C	316	GLN
1	C	331	ASN
1	C	333	ASN
1	D	66	ASN
1	D	118	GLN
1	D	287	GLN
1	D	331	ASN
1	D	404	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

16 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	NAG	E	1	2	15,15,15	2.23	6 (40%)	21,21,21	2.40	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	2	2	14,14,15	2.08	5 (35%)	17,19,21	1.76	4 (23%)
3	GLC	F	1	3	12,12,12	1.93	3 (25%)	17,17,17	1.26	3 (17%)
3	GLC	F	2	3	11,11,12	2.08	4 (36%)	15,15,17	1.47	4 (26%)
2	NAG	G	1	2	15,15,15	2.33	7 (46%)	21,21,21	2.40	7 (33%)
2	NAG	G	2	2	14,14,15	2.14	5 (35%)	17,19,21	1.52	4 (23%)
3	GLC	H	1	3	12,12,12	1.99	3 (25%)	17,17,17	1.06	0
3	GLC	H	2	3	11,11,12	2.03	5 (45%)	15,15,17	1.11	1 (6%)
2	NAG	I	1	2	15,15,15	2.23	6 (40%)	21,21,21	2.23	4 (19%)
2	NAG	I	2	2	14,14,15	2.05	3 (21%)	17,19,21	1.52	4 (23%)
3	GLC	J	1	3	12,12,12	2.03	3 (25%)	17,17,17	1.13	0
3	GLC	J	2	3	11,11,12	2.06	4 (36%)	15,15,17	1.06	1 (6%)
2	NAG	K	1	2	15,15,15	2.24	6 (40%)	21,21,21	2.25	6 (28%)
2	NAG	K	2	2	14,14,15	2.07	5 (35%)	17,19,21	1.60	4 (23%)
3	GLC	L	1	3	12,12,12	1.95	3 (25%)	17,17,17	0.97	0
3	GLC	L	2	3	11,11,12	2.09	5 (45%)	15,15,17	1.10	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	NAG	E	1	2	-	2/6/26/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
3	GLC	F	1	3	-	2/2/22/22	0/1/1/1
3	GLC	F	2	3	-	2/2/19/22	0/1/1/1
2	NAG	G	1	2	-	1/6/26/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
3	GLC	H	1	3	-	0/2/22/22	0/1/1/1
3	GLC	H	2	3	-	2/2/19/22	0/1/1/1
2	NAG	I	1	2	-	2/6/26/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
3	GLC	J	1	3	-	2/2/22/22	0/1/1/1
3	GLC	J	2	3	-	2/2/19/22	0/1/1/1
2	NAG	K	1	2	-	1/6/26/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
3	GLC	L	1	3	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLC	L	2	3	-	0/2/19/22	0/1/1/1

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	NAG	C3-C2	-4.66	1.42	1.52
2	G	2	NAG	C3-C2	-4.64	1.42	1.52
2	I	2	NAG	C3-C2	-4.56	1.42	1.52
3	J	1	GLC	C3-C2	-4.49	1.40	1.52
2	K	2	NAG	C3-C2	-4.44	1.43	1.52
3	H	1	GLC	C3-C2	-4.34	1.41	1.52
2	G	1	NAG	C3-C2	-4.32	1.44	1.53
2	K	1	NAG	C3-C2	-4.20	1.45	1.53
2	E	1	NAG	C3-C2	-4.18	1.45	1.53
3	L	1	GLC	C3-C2	-4.15	1.41	1.52
3	F	1	GLC	C3-C2	-4.08	1.41	1.52
2	E	1	NAG	C4-C3	-4.07	1.42	1.52
2	G	1	NAG	C4-C3	-4.00	1.42	1.52
2	K	1	NAG	C4-C3	-3.94	1.42	1.52
2	I	1	NAG	C3-C2	-3.93	1.45	1.53
2	I	1	NAG	C4-C3	-3.91	1.42	1.52
2	G	1	NAG	C7-N2	3.91	1.47	1.34
2	I	1	NAG	C7-N2	3.80	1.47	1.34
3	H	1	GLC	C4-C3	-3.80	1.42	1.52
2	K	1	NAG	C7-N2	3.79	1.47	1.34
3	J	1	GLC	C4-C3	-3.78	1.42	1.52
2	E	1	NAG	C7-N2	3.75	1.47	1.34
3	L	1	GLC	C4-C3	-3.75	1.42	1.52
3	F	1	GLC	C4-C3	-3.65	1.43	1.52
3	H	2	GLC	C4-C3	-3.57	1.43	1.52
3	F	2	GLC	O5-C1	-3.57	1.38	1.43
3	L	2	GLC	C4-C3	-3.55	1.43	1.52
3	F	2	GLC	C4-C3	-3.48	1.43	1.52
3	J	2	GLC	C4-C3	-3.46	1.43	1.52
3	J	2	GLC	O5-C1	-3.41	1.38	1.43
2	I	2	NAG	O5-C1	3.39	1.49	1.43
2	G	2	NAG	O5-C1	3.30	1.49	1.43
2	K	2	NAG	O5-C1	3.26	1.48	1.43
2	G	2	NAG	C7-N2	3.25	1.45	1.34
2	G	1	NAG	C1-C2	-3.17	1.49	1.52
3	L	2	GLC	O5-C1	-3.14	1.38	1.43
2	K	2	NAG	C7-N2	3.13	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1	NAG	C1-C2	-3.11	1.49	1.52
2	E	2	NAG	O5-C1	3.07	1.48	1.43
3	H	2	GLC	O5-C1	-3.01	1.38	1.43
2	E	2	NAG	C7-N2	3.00	1.44	1.34
2	I	2	NAG	C7-N2	2.93	1.44	1.34
2	I	1	NAG	C1-C2	-2.84	1.49	1.52
3	L	2	GLC	O5-C5	2.79	1.49	1.43
3	H	2	GLC	O5-C5	2.79	1.49	1.43
2	E	1	NAG	C1-C2	-2.77	1.49	1.52
3	F	2	GLC	O5-C5	2.63	1.48	1.43
3	J	2	GLC	O5-C5	2.61	1.48	1.43
3	J	2	GLC	C2-C3	-2.57	1.48	1.52
3	L	2	GLC	C2-C3	-2.56	1.48	1.52
3	F	2	GLC	C2-C3	-2.49	1.48	1.52
2	I	1	NAG	O3-C3	2.41	1.48	1.43
3	H	2	GLC	C2-C3	-2.24	1.49	1.52
2	G	2	NAG	O5-C5	-2.23	1.38	1.43
3	F	1	GLC	O3-C3	2.22	1.48	1.43
2	I	1	NAG	O4-C4	2.22	1.48	1.43
2	G	1	NAG	O3-C3	2.22	1.48	1.43
3	H	1	GLC	O3-C3	2.19	1.48	1.43
2	G	1	NAG	O4-C4	2.19	1.48	1.43
3	L	1	GLC	O3-C3	2.14	1.48	1.43
2	K	2	NAG	C1-C2	-2.13	1.49	1.52
2	K	1	NAG	O4-C4	2.12	1.48	1.43
3	H	2	GLC	O3-C3	2.09	1.47	1.43
2	G	2	NAG	C2-N2	2.08	1.49	1.46
3	J	1	GLC	O3-C3	2.08	1.47	1.43
2	E	1	NAG	O4-C4	2.07	1.47	1.43
2	K	1	NAG	O3-C3	2.06	1.47	1.43
2	E	2	NAG	C1-C2	-2.05	1.49	1.52
2	G	1	NAG	C2-N2	2.05	1.49	1.45
3	L	2	GLC	O3-C3	2.05	1.47	1.43
2	E	2	NAG	O5-C5	-2.03	1.39	1.43
2	E	1	NAG	O3-C3	2.03	1.47	1.43
2	K	2	NAG	O5-C5	-2.00	1.39	1.43

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	C1-C2-N2	6.94	118.76	110.73
2	I	1	NAG	C1-C2-N2	5.66	117.28	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	NAG	C1-C2-N2	5.30	116.87	110.73
2	I	1	NAG	O5-C5-C4	5.22	119.18	109.69
2	K	1	NAG	C1-C2-C3	-5.18	103.48	110.54
2	K	1	NAG	O5-C5-C4	4.67	118.17	109.69
2	E	1	NAG	C1-C2-C3	-4.64	104.22	110.54
2	K	1	NAG	C1-C2-N2	4.51	115.96	110.73
2	G	1	NAG	O5-C5-C4	4.50	117.86	109.69
2	G	1	NAG	C1-C2-C3	-4.46	104.46	110.54
2	E	1	NAG	O5-C5-C4	4.30	117.51	109.69
2	E	2	NAG	C1-O5-C5	4.10	117.75	112.19
2	G	1	NAG	C4-C3-C2	-4.09	104.35	110.34
2	K	2	NAG	C2-N2-C7	-4.01	117.19	122.90
2	I	1	NAG	C1-C2-C3	-3.85	105.29	110.54
2	G	2	NAG	C1-O5-C5	3.31	116.68	112.19
2	E	2	NAG	C2-N2-C7	-3.18	118.38	122.90
2	E	2	NAG	C6-C5-C4	-3.01	105.94	113.00
2	I	2	NAG	C2-N2-C7	-3.00	118.63	122.90
2	I	2	NAG	C1-O5-C5	2.96	116.20	112.19
2	E	1	NAG	C4-C3-C2	-2.86	106.15	110.34
2	G	1	NAG	C3-C2-N2	2.82	115.95	110.62
3	F	2	GLC	O5-C5-C6	2.67	111.39	107.20
2	G	2	NAG	C2-N2-C7	-2.63	119.15	122.90
2	G	2	NAG	C8-C7-N2	2.63	120.56	116.10
3	H	2	GLC	O5-C5-C6	2.63	111.33	107.20
3	F	1	GLC	C4-C3-C2	2.60	115.36	110.82
2	K	1	NAG	C3-C2-N2	2.59	115.51	110.62
2	K	1	NAG	C4-C3-C2	-2.56	106.58	110.34
2	E	1	NAG	O1-C1-C2	2.51	114.44	109.22
2	K	2	NAG	C8-C7-N2	2.46	120.27	116.10
2	I	2	NAG	C6-C5-C4	-2.45	107.26	113.00
2	E	2	NAG	C8-C7-N2	2.43	120.21	116.10
2	I	2	NAG	C8-C7-N2	2.39	120.14	116.10
3	F	2	GLC	C1-C2-C3	2.34	112.55	109.67
2	G	1	NAG	O5-C1-C2	2.32	111.84	109.52
2	K	1	NAG	O5-C1-C2	2.30	111.83	109.52
3	J	2	GLC	O5-C5-C6	2.22	110.69	107.20
3	F	1	GLC	O5-C5-C4	2.19	113.67	109.69
2	K	2	NAG	C6-C5-C4	-2.18	107.89	113.00
3	F	1	GLC	O6-C6-C5	2.17	118.72	111.29
3	F	2	GLC	C3-C4-C5	2.12	114.03	110.24
2	I	1	NAG	O6-C6-C5	2.12	118.56	111.29
2	K	2	NAG	O6-C6-C5	2.10	118.50	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	NAG	O6-C6-C5	2.08	118.42	111.29
3	F	2	GLC	O5-C1-C2	2.06	113.95	110.77
3	L	2	GLC	O6-C6-C5	2.04	118.29	111.29
2	G	1	NAG	O6-C6-C5	2.04	118.27	111.29

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C1-C2-N2-C7
2	G	1	NAG	C1-C2-N2-C7
2	I	1	NAG	C1-C2-N2-C7
2	K	1	NAG	C1-C2-N2-C7
3	J	1	GLC	O5-C5-C6-O6
3	J	2	GLC	O5-C5-C6-O6
3	F	2	GLC	O5-C5-C6-O6
3	H	2	GLC	O5-C5-C6-O6
3	F	2	GLC	C4-C5-C6-O6
3	H	2	GLC	C4-C5-C6-O6
3	J	2	GLC	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
3	F	1	GLC	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
3	J	1	GLC	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
3	F	1	GLC	O5-C5-C6-O6

There are no ring outliers.

14 monomers are involved in 32 short contacts:

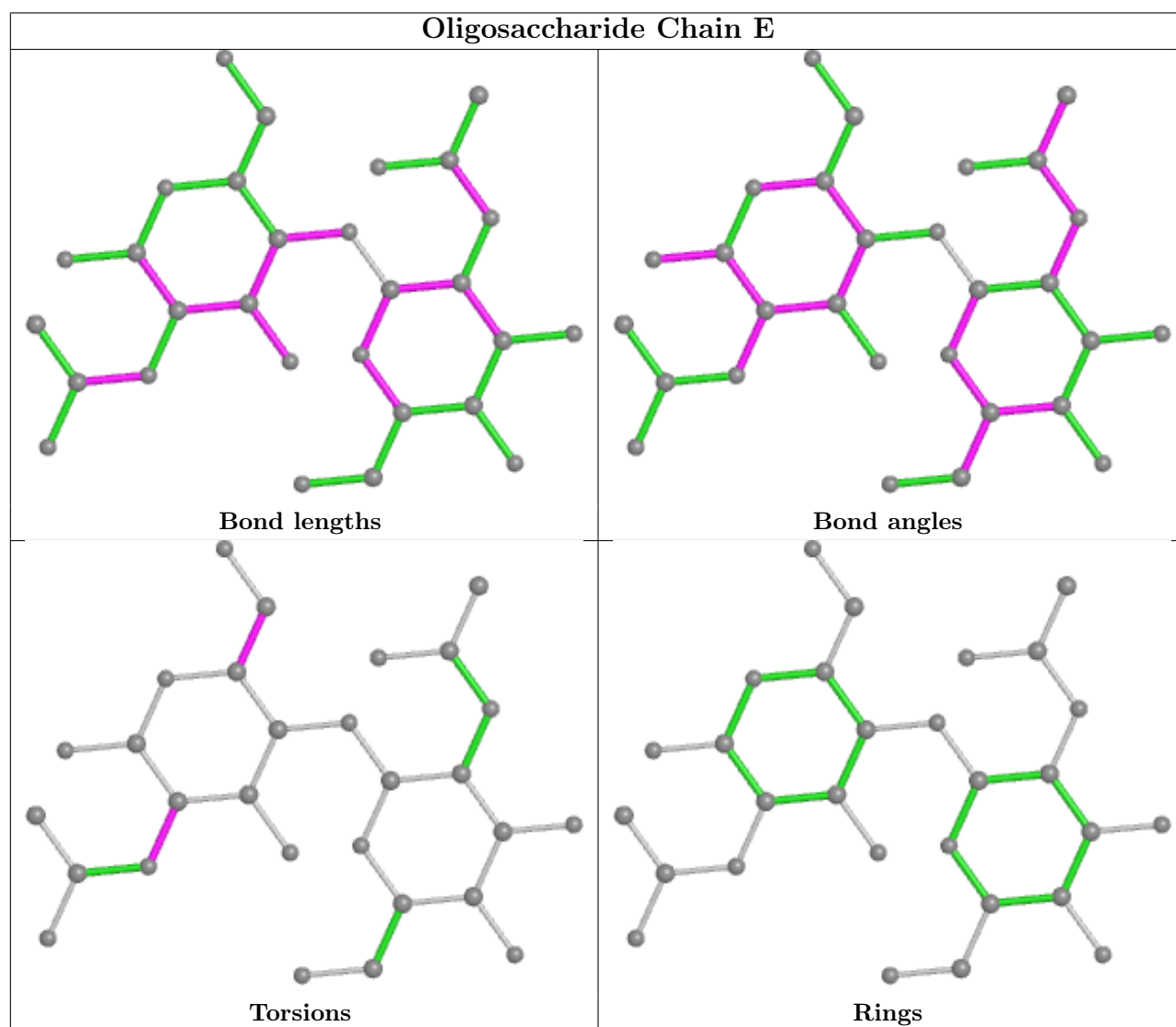
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	2	GLC	1	0
3	F	2	GLC	2	0
3	J	2	GLC	1	0
3	L	1	GLC	1	0
2	I	2	NAG	5	0
2	G	1	NAG	2	0
2	G	2	NAG	4	0

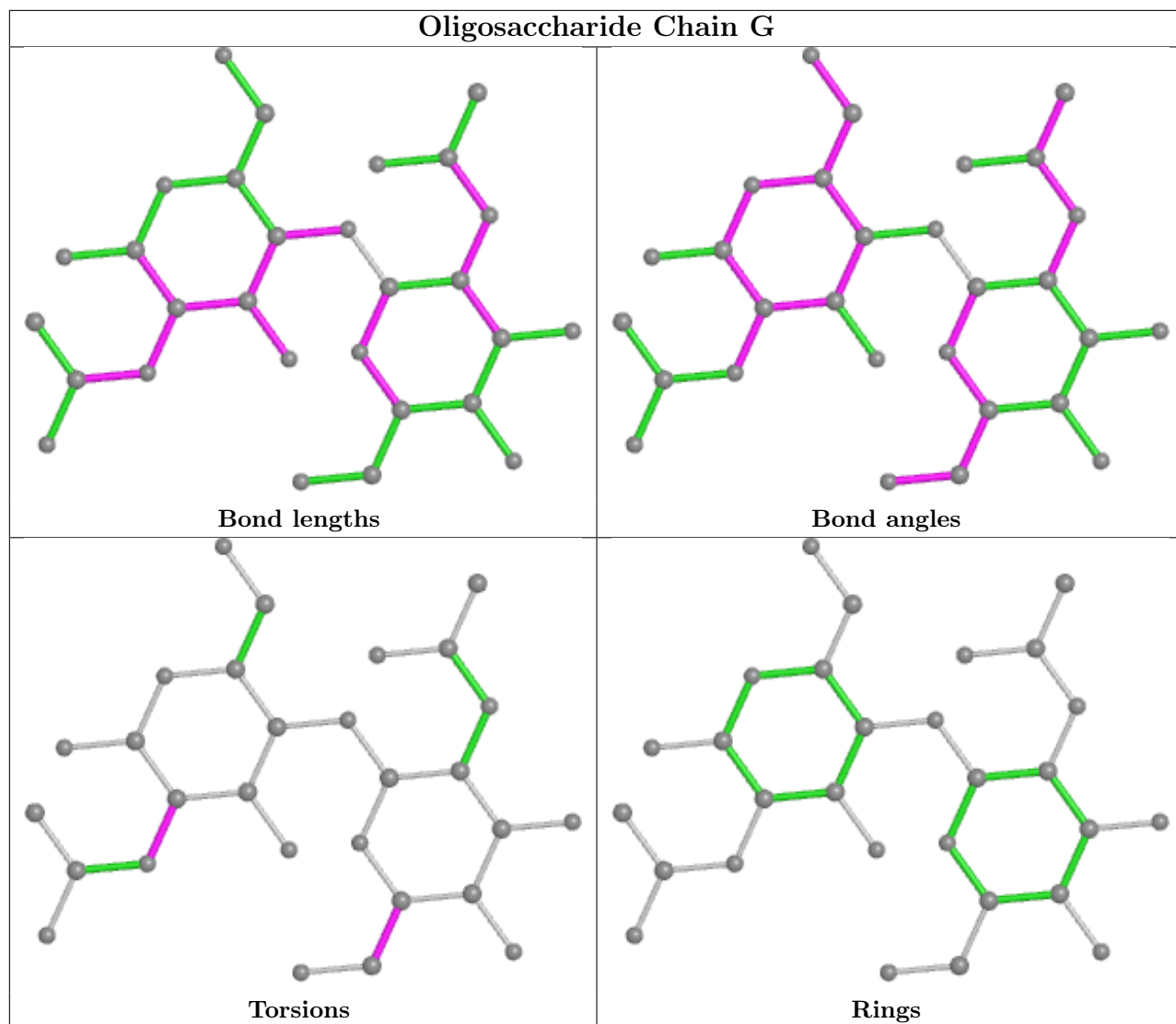
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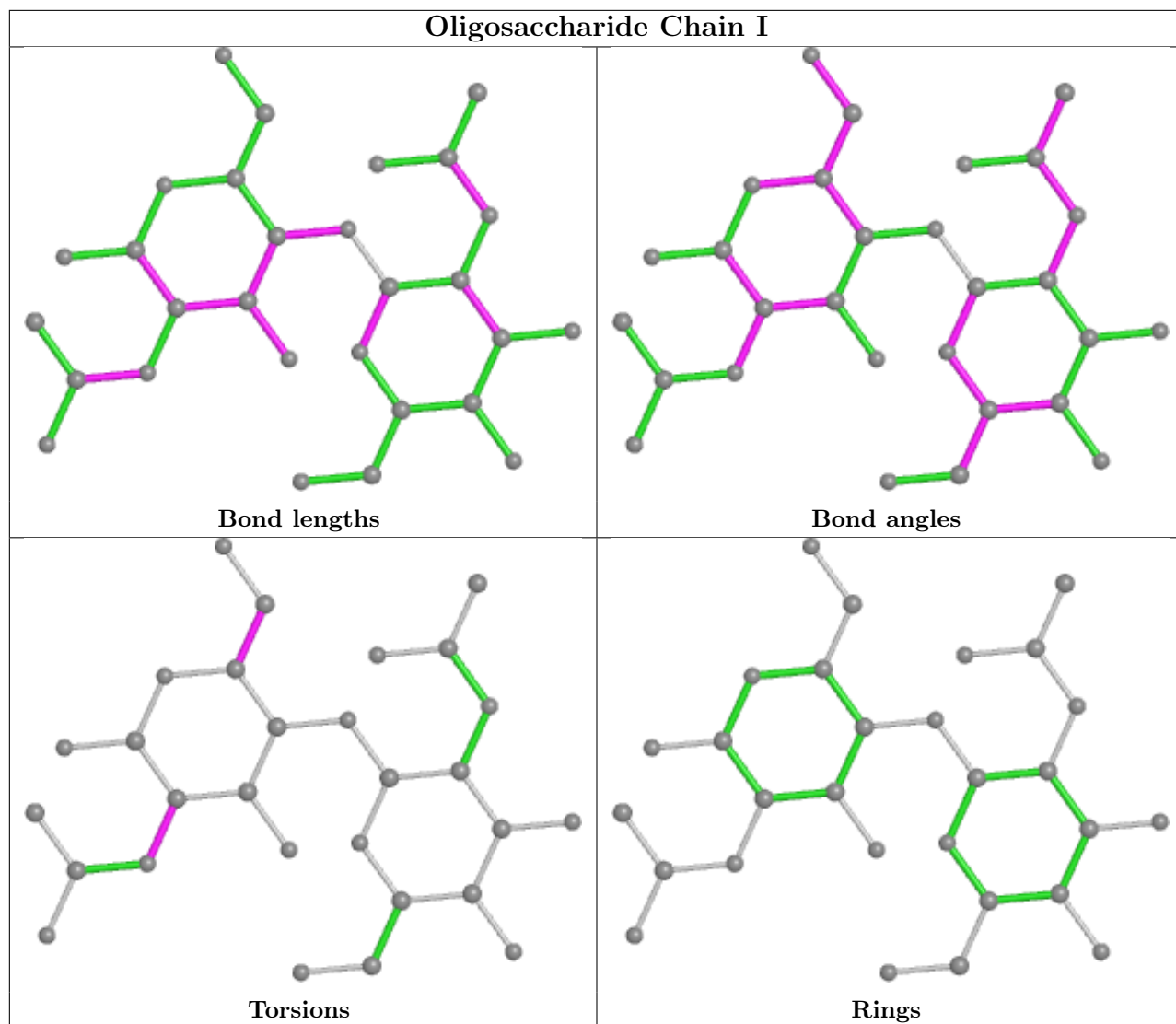
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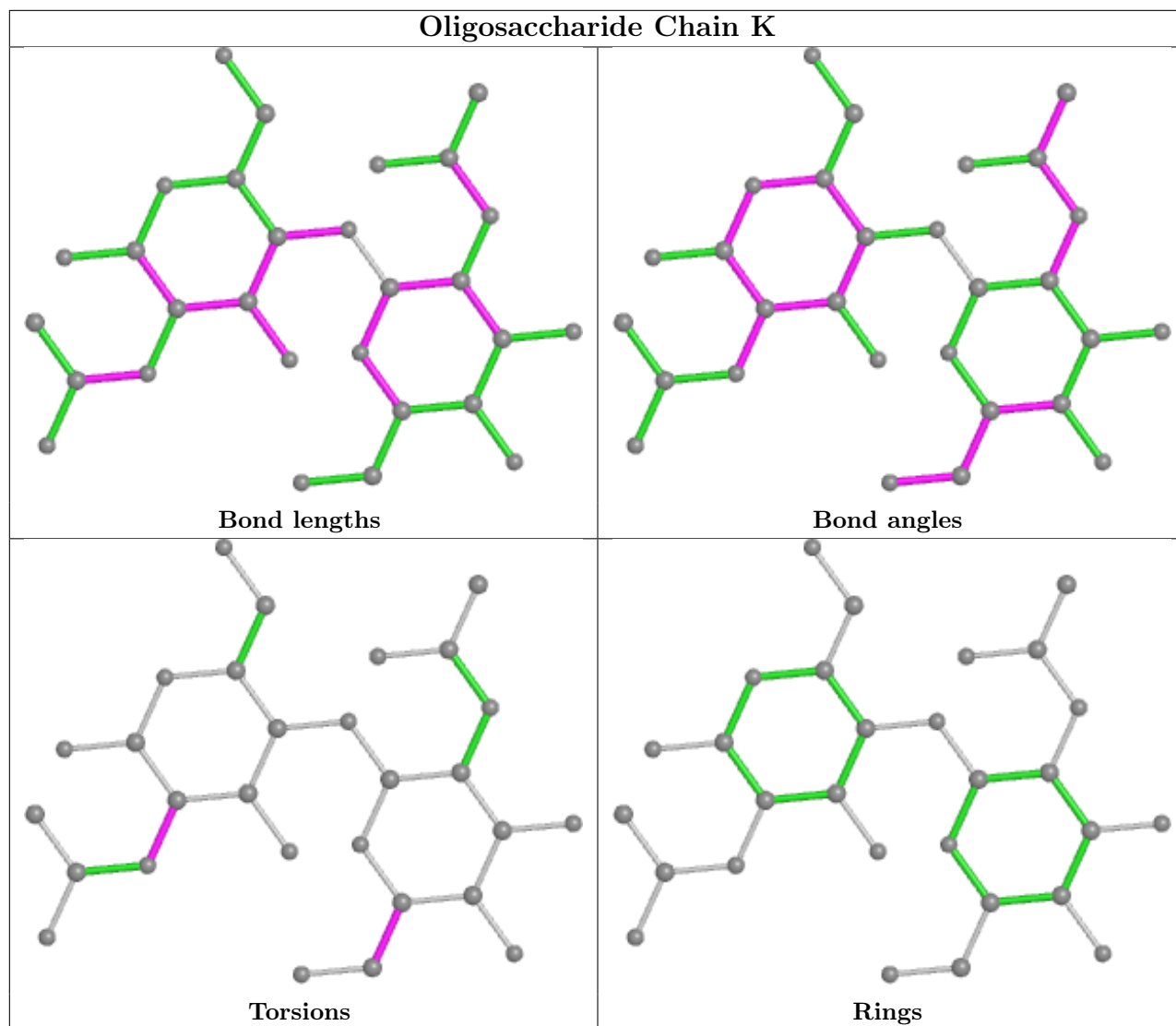
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	4	0
2	E	2	NAG	2	0
2	I	1	NAG	3	0
2	K	1	NAG	3	0
3	J	1	GLC	2	0
2	K	2	NAG	3	0
3	F	1	GLC	3	0

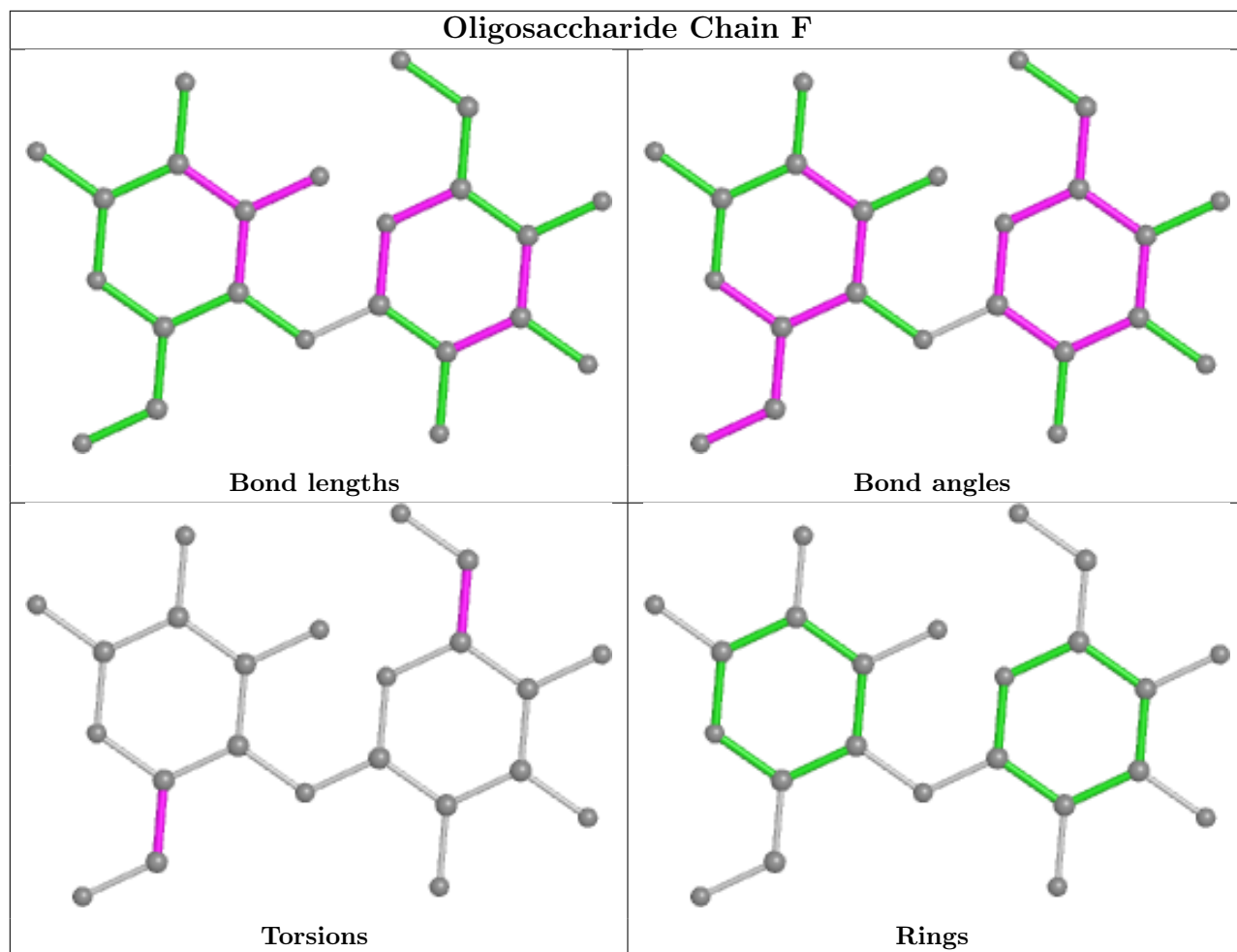
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

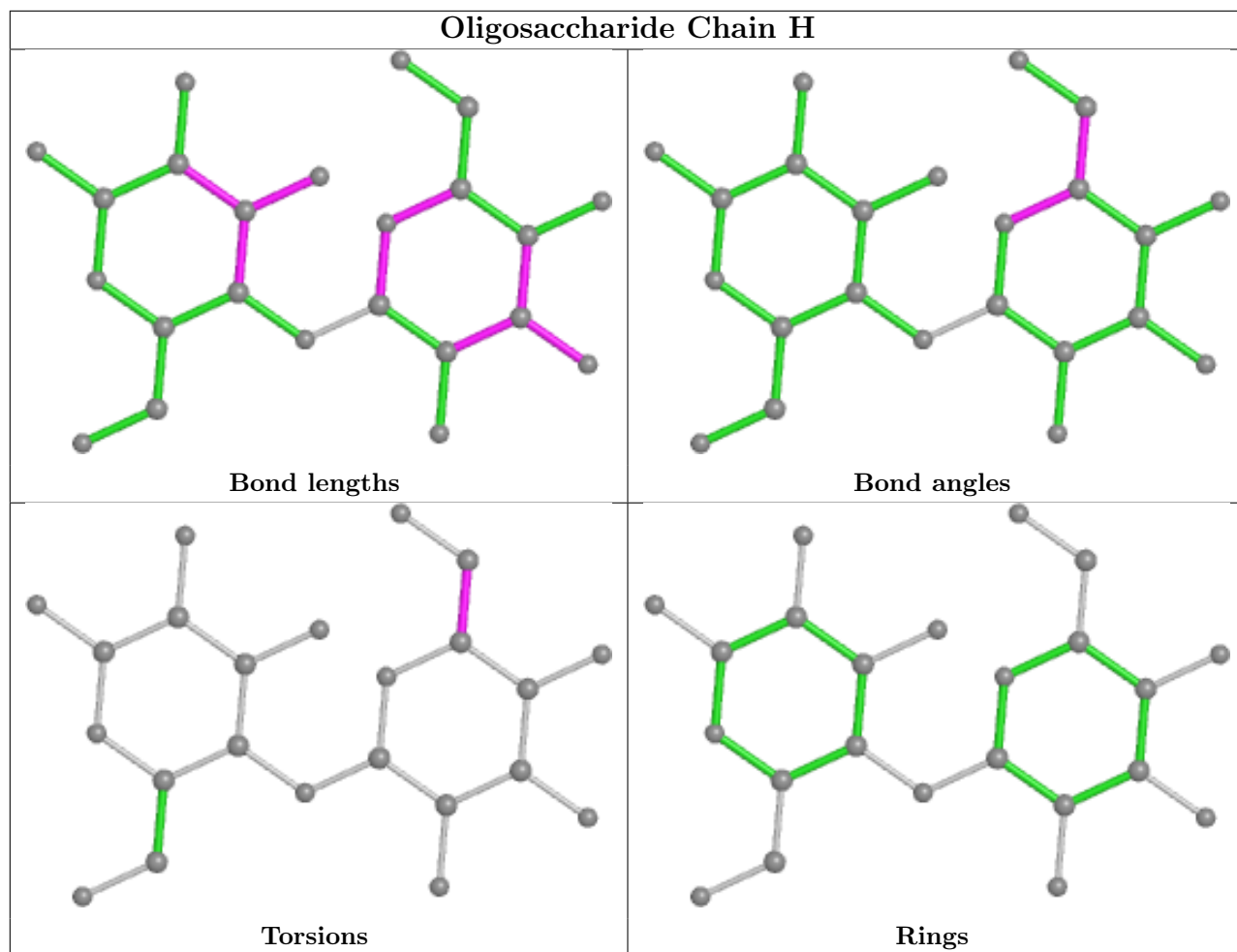


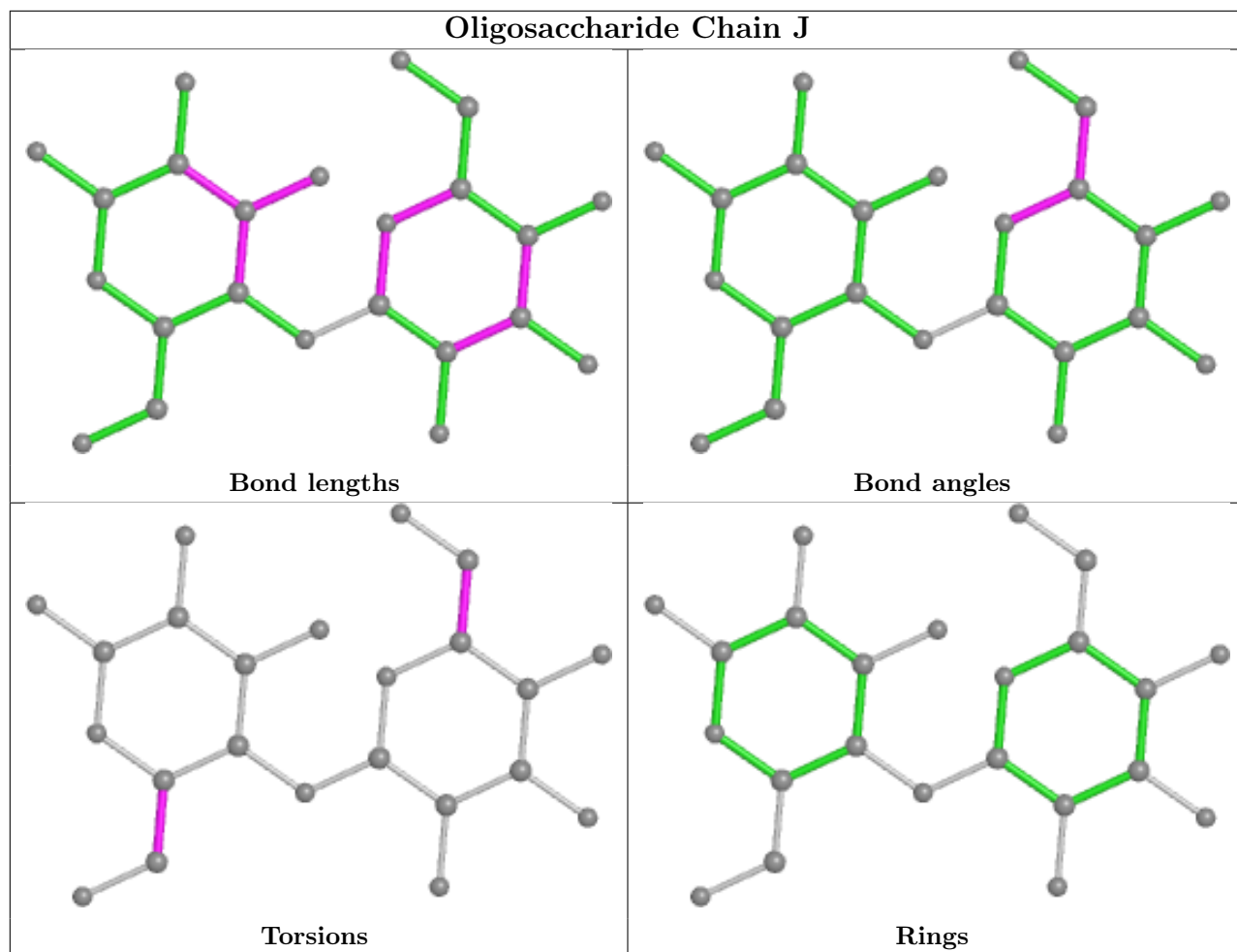


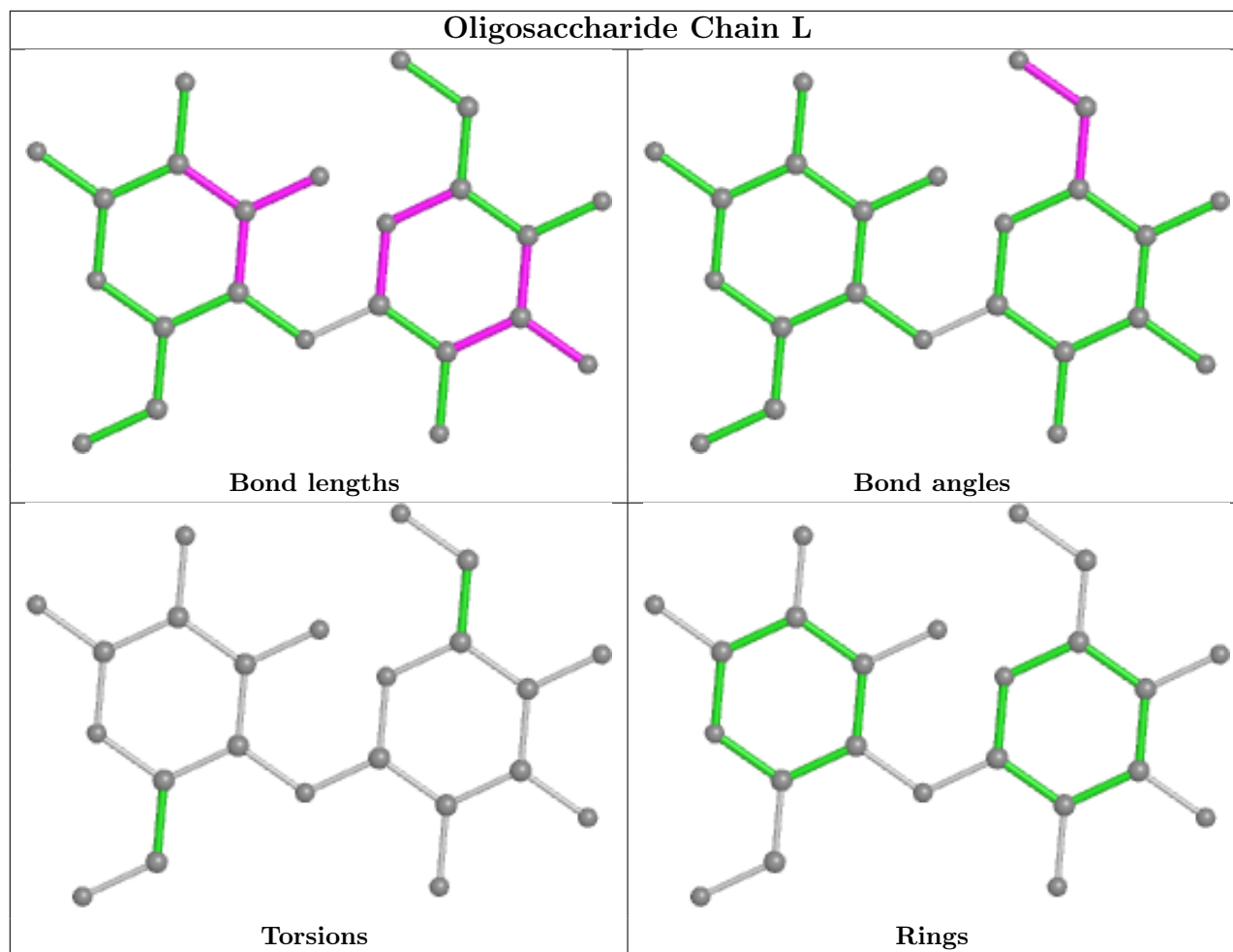












5.6 Ligand geometry [i](#)

11 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$
4	ZDM	C	600	-	31,31,33	1.60	6 (19%)	42,42,44	1.57	6 (14%)
5	CIT	C	444	-	12,12,12	0.96	0	17,17,17	1.48	2 (11%)
5	CIT	C	445	-	12,12,12	0.98	0	17,17,17	1.63	4 (23%)
4	ZDM	A	600	-	31,31,33	1.68	8 (25%)	42,42,44	1.48	4 (9%)
5	CIT	B	443	-	12,12,12	0.98	0	17,17,17	1.54	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ZDM	A	443	-	31,31,33	1.66	7 (22%)	42,42,44	1.91	14 (33%)
5	CIT	B	800	-	12,12,12	0.96	0	17,17,17	1.58	4 (23%)
5	CIT	D	800	-	12,12,12	0.97	0	17,17,17	1.55	4 (23%)
5	CIT	C	800	-	12,12,12	1.02	0	17,17,17	1.73	4 (23%)
5	CIT	A	444	-	12,12,12	1.10	0	17,17,17	1.75	6 (35%)
4	ZDM	C	443	-	31,31,33	1.61	5 (16%)	42,42,44	1.73	13 (30%)

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	ZDM	C	600	-	-	10/16/56/58	0/2/2/2
5	CIT	C	444	-	-	10/16/16/16	-
5	CIT	C	445	-	-	9/16/16/16	-
4	ZDM	A	600	-	-	10/16/56/58	0/2/2/2
5	CIT	B	443	-	-	7/16/16/16	-
4	ZDM	A	443	-	-	7/16/56/58	0/2/2/2
5	CIT	B	800	-	-	10/16/16/16	-
5	CIT	D	800	-	-	7/16/16/16	-
5	CIT	C	800	-	-	11/16/16/16	-
5	CIT	A	444	-	-	7/16/16/16	-
4	ZDM	C	443	-	-	12/16/56/58	0/2/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	443	ZDM	C8-C7	-4.76	1.40	1.52
4	C	443	ZDM	C8-C7	-4.61	1.40	1.52
4	A	600	ZDM	C8-C7	-4.58	1.40	1.52
4	C	600	ZDM	C8-C7	-4.51	1.40	1.52
4	A	600	ZDM	C2-C3	-3.93	1.41	1.52
4	C	600	ZDM	C2-C3	-3.92	1.41	1.52
4	C	443	ZDM	C2-C3	-3.82	1.42	1.52
4	A	443	ZDM	C2-C3	-3.76	1.42	1.52
4	A	600	ZDM	C7-C5	-2.67	1.45	1.52
4	A	443	ZDM	C7-C5	-2.62	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	600	ZDM	C7-C5	-2.60	1.45	1.52
4	C	443	ZDM	C7-C5	-2.59	1.45	1.52
4	A	443	ZDM	C8-C9	-2.45	1.47	1.53
4	C	443	ZDM	O5-C4	2.41	1.50	1.44
4	A	600	ZDM	C8-C9	-2.41	1.48	1.53
4	A	600	ZDM	O7-C3	2.38	1.50	1.43
4	C	443	ZDM	O4-C7	2.32	1.48	1.43
4	A	600	ZDM	O5-C4	2.29	1.49	1.44
4	C	600	ZDM	O4-C7	2.21	1.48	1.43
4	C	600	ZDM	O7-C3	2.15	1.49	1.43
4	C	600	ZDM	O5-C4	2.14	1.49	1.44
4	A	443	ZDM	O7-C3	2.12	1.49	1.43
4	A	443	ZDM	O4-C7	2.12	1.48	1.43
4	A	600	ZDM	C2-C1	-2.11	1.47	1.52
4	A	443	ZDM	O5-C4	2.10	1.49	1.44
4	A	600	ZDM	O4-C7	2.05	1.47	1.43

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	443	ZDM	C18-O16-C6	5.61	123.14	113.84
4	C	600	ZDM	C18-O16-C6	5.49	122.95	113.84
4	C	443	ZDM	C18-O16-C6	4.83	121.84	113.84
5	C	800	CIT	O6-C6-C3	4.72	121.25	113.05
4	A	600	ZDM	C18-O16-C6	4.63	121.51	113.84
5	C	445	CIT	O6-C6-C3	4.18	120.30	113.05
5	D	800	CIT	O6-C6-C3	4.04	120.06	113.05
5	B	800	CIT	O6-C6-C3	3.88	119.79	113.05
5	B	443	CIT	O6-C6-C3	3.87	119.77	113.05
5	C	444	CIT	O6-C6-C3	3.70	119.48	113.05
4	A	600	ZDM	O7-C3-C2	3.66	117.02	107.28
4	A	443	ZDM	O1-C10-C5	3.60	117.96	110.35
4	A	443	ZDM	O16-C6-C1	3.58	113.89	108.30
5	A	444	CIT	O6-C6-C3	3.47	119.07	113.05
4	C	443	ZDM	O16-C6-C1	3.02	113.01	108.30
5	A	444	CIT	C3-C2-C1	2.88	120.78	113.81
4	C	600	ZDM	O5-C4-C3	2.83	115.72	109.75
4	A	443	ZDM	O16-C18-C19	2.77	119.27	109.56
4	C	443	ZDM	O1-C10-C5	2.73	116.12	110.35
4	C	600	ZDM	O1-C10-C5	2.70	116.06	110.35
4	A	443	ZDM	C10-C5-C7	2.69	115.61	110.00
4	A	600	ZDM	O5-C4-C3	2.69	115.42	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	443	ZDM	O7-C3-C2	2.65	114.32	107.28
4	A	443	ZDM	O49-C1-C2	-2.57	104.41	110.35
4	A	600	ZDM	O16-C18-C19	2.55	118.50	109.56
4	C	443	ZDM	O16-C18-C19	2.48	118.25	109.56
4	A	443	ZDM	C10-O7-C3	-2.47	111.84	117.96
4	C	600	ZDM	O16-C18-C19	2.45	118.15	109.56
5	A	444	CIT	C2-C3-C6	2.45	115.37	110.11
4	C	443	ZDM	O2-C8-C9	2.45	115.37	109.30
4	A	443	ZDM	O7-C3-C2	2.41	113.69	107.28
4	A	443	ZDM	O49-C1-C6	2.40	115.86	110.05
4	C	600	ZDM	C10-O7-C3	-2.37	112.11	117.96
4	A	443	ZDM	O1-C9-C11	2.34	112.26	106.44
5	C	445	CIT	O4-C5-C4	2.30	121.73	114.35
5	A	444	CIT	C4-C3-C6	-2.27	105.24	110.11
4	C	443	ZDM	C10-C5-C7	2.24	114.66	110.00
5	B	800	CIT	O2-C1-C2	2.24	121.55	114.35
4	C	443	ZDM	O3-C5-C10	2.22	115.43	110.05
4	A	443	ZDM	O3-C5-C10	2.20	115.38	110.05
4	C	443	ZDM	O7-C10-C5	2.19	113.77	108.10
5	A	444	CIT	O2-C1-C2	2.17	121.31	114.35
4	C	443	ZDM	C6-O5-C4	-2.17	109.44	113.69
5	B	443	CIT	O2-C1-O1	-2.16	117.92	123.30
5	B	443	CIT	O4-C5-C4	2.15	121.27	114.35
5	C	800	CIT	O2-C1-C2	2.15	121.25	114.35
4	C	443	ZDM	C2-C3-C4	-2.15	106.01	110.93
4	A	443	ZDM	O2-C8-C7	2.13	115.27	110.35
5	A	444	CIT	O2-C1-O1	-2.11	118.03	123.30
4	A	443	ZDM	O7-C10-C5	2.11	113.58	108.10
4	C	600	ZDM	O1-C9-C11	2.11	111.68	106.44
5	C	800	CIT	O2-C1-O1	-2.10	118.06	123.30
5	C	444	CIT	O4-C5-C4	2.10	121.09	114.35
5	D	800	CIT	O2-C1-C2	2.10	121.08	114.35
5	B	800	CIT	O4-C5-C4	2.09	121.07	114.35
5	C	445	CIT	O2-C1-O1	-2.08	118.11	123.30
5	D	800	CIT	O4-C5-C4	2.07	120.99	114.35
5	B	800	CIT	O2-C1-O1	-2.06	118.17	123.30
5	C	445	CIT	O2-C1-C2	2.05	120.95	114.35
4	C	443	ZDM	O6-C11-C9	2.05	118.32	111.29
5	B	443	CIT	O2-C1-C2	2.03	120.86	114.35
5	D	800	CIT	O2-C1-O1	-2.02	118.26	123.30
5	C	800	CIT	O4-C5-C4	2.02	120.84	114.35
4	C	443	ZDM	O5-C4-C3	2.01	114.00	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	443	ZDM	O55-C2-C1	-2.01	105.70	110.35

There are no chirality outliers.

All (100) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	600	ZDM	C1-C6-O16-C18
4	A	600	ZDM	O5-C6-O16-C18
4	C	443	ZDM	C1-C6-O16-C18
4	C	443	ZDM	O5-C6-O16-C18
4	C	600	ZDM	C1-C6-O16-C18
4	C	600	ZDM	O5-C6-O16-C18
5	A	444	CIT	C2-C3-C4-C5
5	A	444	CIT	O7-C3-C4-C5
5	A	444	CIT	C6-C3-C4-C5
5	A	444	CIT	C2-C3-C6-O5
5	A	444	CIT	C2-C3-C6-O6
5	A	444	CIT	O7-C3-C6-O5
5	A	444	CIT	O7-C3-C6-O6
5	B	443	CIT	C2-C3-C6-O5
5	B	443	CIT	C2-C3-C6-O6
5	B	443	CIT	O7-C3-C6-O5
5	B	443	CIT	O7-C3-C6-O6
5	B	800	CIT	C2-C3-C6-O5
5	B	800	CIT	C2-C3-C6-O6
5	B	800	CIT	O7-C3-C6-O5
5	B	800	CIT	O7-C3-C6-O6
5	C	444	CIT	C1-C2-C3-O7
5	C	444	CIT	C1-C2-C3-C4
5	C	444	CIT	C1-C2-C3-C6
5	C	444	CIT	O7-C3-C6-O5
5	C	444	CIT	O7-C3-C6-O6
5	C	444	CIT	C4-C3-C6-O5
5	C	444	CIT	C4-C3-C6-O6
5	C	800	CIT	C1-C2-C3-O7
5	C	800	CIT	C1-C2-C3-C6
5	C	800	CIT	C2-C3-C6-O5
5	C	800	CIT	C2-C3-C6-O6
5	C	800	CIT	O7-C3-C6-O5
5	C	800	CIT	O7-C3-C6-O6
5	D	800	CIT	C2-C3-C6-O5
5	D	800	CIT	C2-C3-C6-O6

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Mol	Chain	Res	Type	Atoms
5	D	800	CIT	O7-C3-C6-O5
5	D	800	CIT	O7-C3-C6-O6
4	C	443	ZDM	O6-C11-C9-O1
4	C	600	ZDM	O6-C11-C9-C8
4	C	443	ZDM	O6-C11-C9-C8
5	C	800	CIT	C1-C2-C3-C4
4	C	600	ZDM	O6-C11-C9-O1
5	D	800	CIT	O7-C3-C4-C5
4	A	443	ZDM	C1-C6-O16-C18
4	C	443	ZDM	O16-C18-C19-C22
4	A	600	ZDM	C4-C3-O7-C10
4	A	600	ZDM	O16-C18-C19-C22
4	C	600	ZDM	C18-C19-C22-C25
4	C	443	ZDM	C18-C19-C22-C25
4	A	600	ZDM	C2-C3-O7-C10
4	C	600	ZDM	O16-C18-C19-C22
5	B	800	CIT	C1-C2-C3-C6
5	D	800	CIT	C6-C3-C4-C5
4	C	443	ZDM	C5-C10-O7-C3
4	C	600	ZDM	C2-C3-O7-C10
4	C	600	ZDM	C4-C3-O7-C10
4	A	600	ZDM	C25-C28-C31-C34
5	B	443	CIT	O7-C3-C4-C5
5	B	800	CIT	C1-C2-C3-O7
5	B	800	CIT	O7-C3-C4-C5
5	D	800	CIT	C2-C3-C4-C5
4	A	443	ZDM	C5-C10-O7-C3
5	C	445	CIT	C2-C3-C6-O5
5	C	445	CIT	C2-C3-C6-O6
5	C	445	CIT	C4-C3-C6-O5
5	C	445	CIT	C4-C3-C6-O6
4	A	443	ZDM	O16-C18-C19-C22
5	B	443	CIT	C6-C3-C4-C5
5	B	800	CIT	C6-C3-C4-C5
5	C	800	CIT	C6-C3-C4-C5
4	A	443	ZDM	O5-C6-O16-C18
5	C	444	CIT	C6-C3-C4-C5
5	B	800	CIT	C1-C2-C3-C4
4	C	600	ZDM	C19-C22-C25-C28
4	A	600	ZDM	C22-C25-C28-C31
4	C	443	ZDM	C25-C28-C31-C34
5	B	443	CIT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
5	C	444	CIT	O7-C3-C4-C5
5	C	800	CIT	O7-C3-C4-C5
4	C	443	ZDM	C22-C25-C28-C31
4	A	600	ZDM	C18-C19-C22-C25
4	A	443	ZDM	O5-C4-C57-O61
4	C	443	ZDM	C4-C3-O7-C10
5	B	800	CIT	C2-C3-C4-C5
5	C	444	CIT	C2-C3-C4-C5
4	C	600	ZDM	C25-C28-C31-C34
5	C	445	CIT	O7-C3-C6-O5
5	C	445	CIT	O7-C3-C6-O6
4	A	600	ZDM	O6-C11-C9-C8
4	A	443	ZDM	C22-C25-C28-C31
5	C	445	CIT	C3-C4-C5-O4
4	C	443	ZDM	O1-C10-O7-C3
4	C	443	ZDM	C2-C3-O7-C10
5	C	445	CIT	C2-C3-C4-C5
5	C	445	CIT	C3-C4-C5-O3
5	C	800	CIT	C3-C4-C5-O3
4	A	443	ZDM	C4-C3-O7-C10
5	C	800	CIT	C3-C4-C5-O4
4	A	600	ZDM	O6-C11-C9-O1

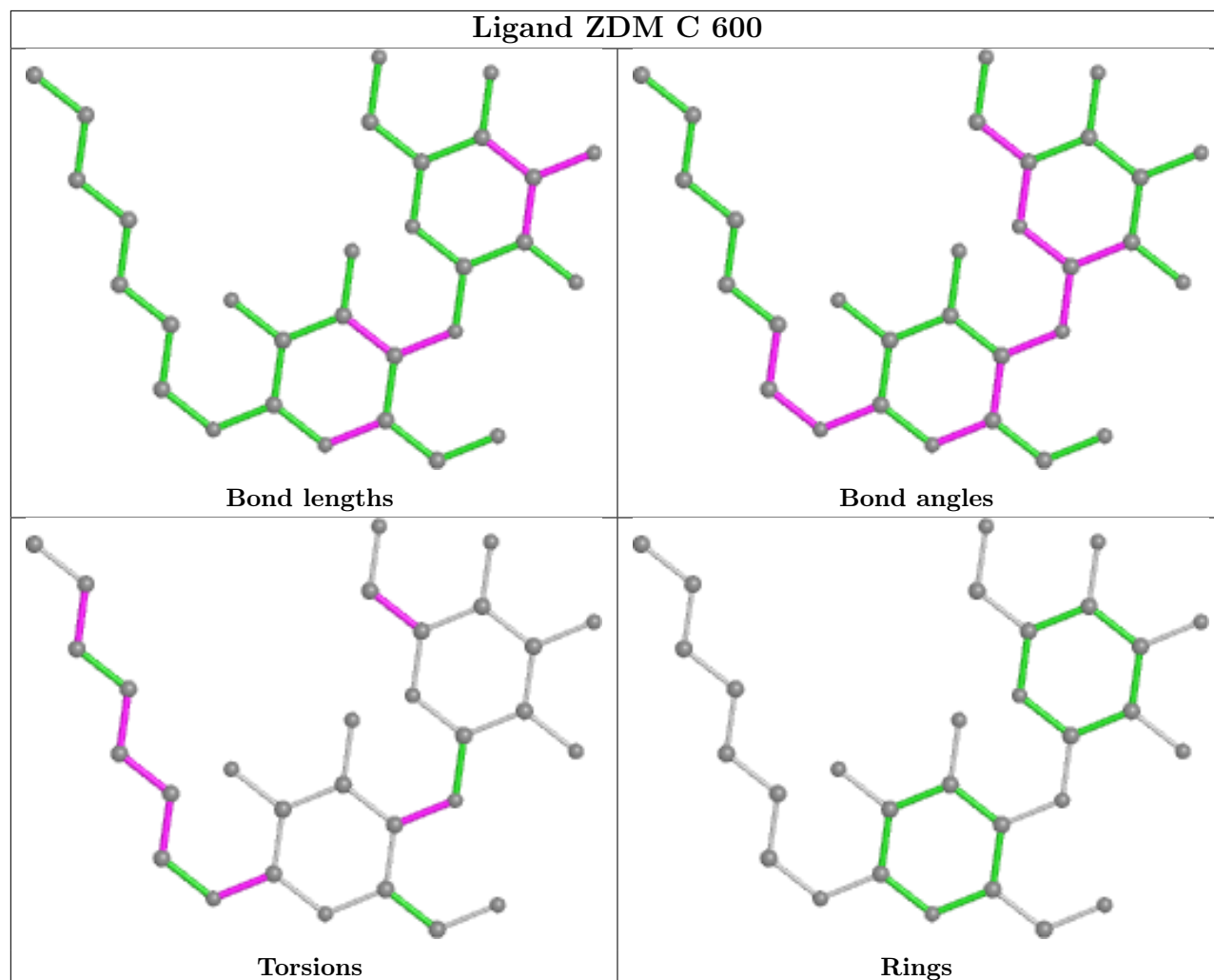
There are no ring outliers.

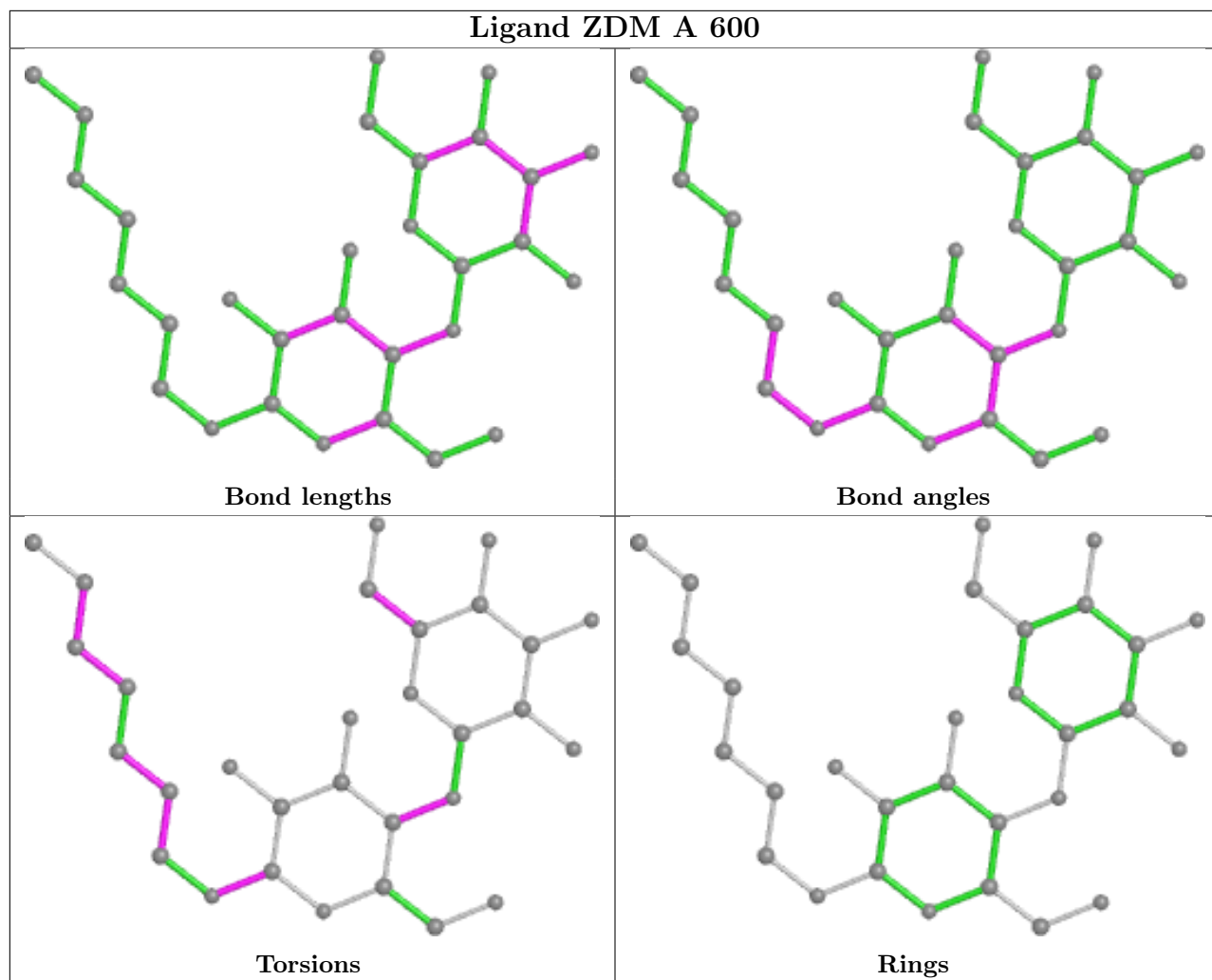
5 monomers are involved in 29 short contacts:

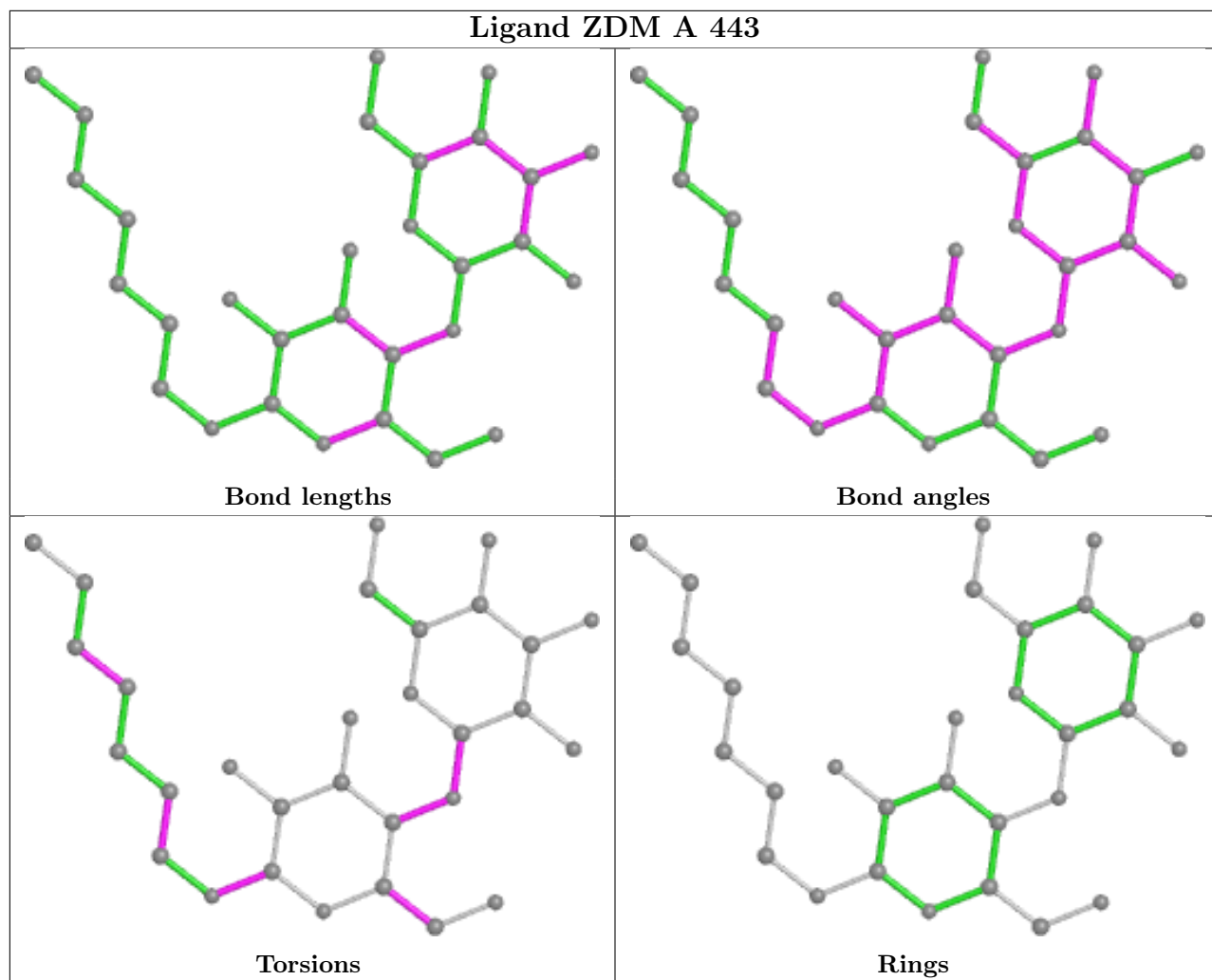
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	600	ZDM	7	0
5	C	444	CIT	1	0
4	A	600	ZDM	7	0
4	A	443	ZDM	8	0
4	C	443	ZDM	6	0

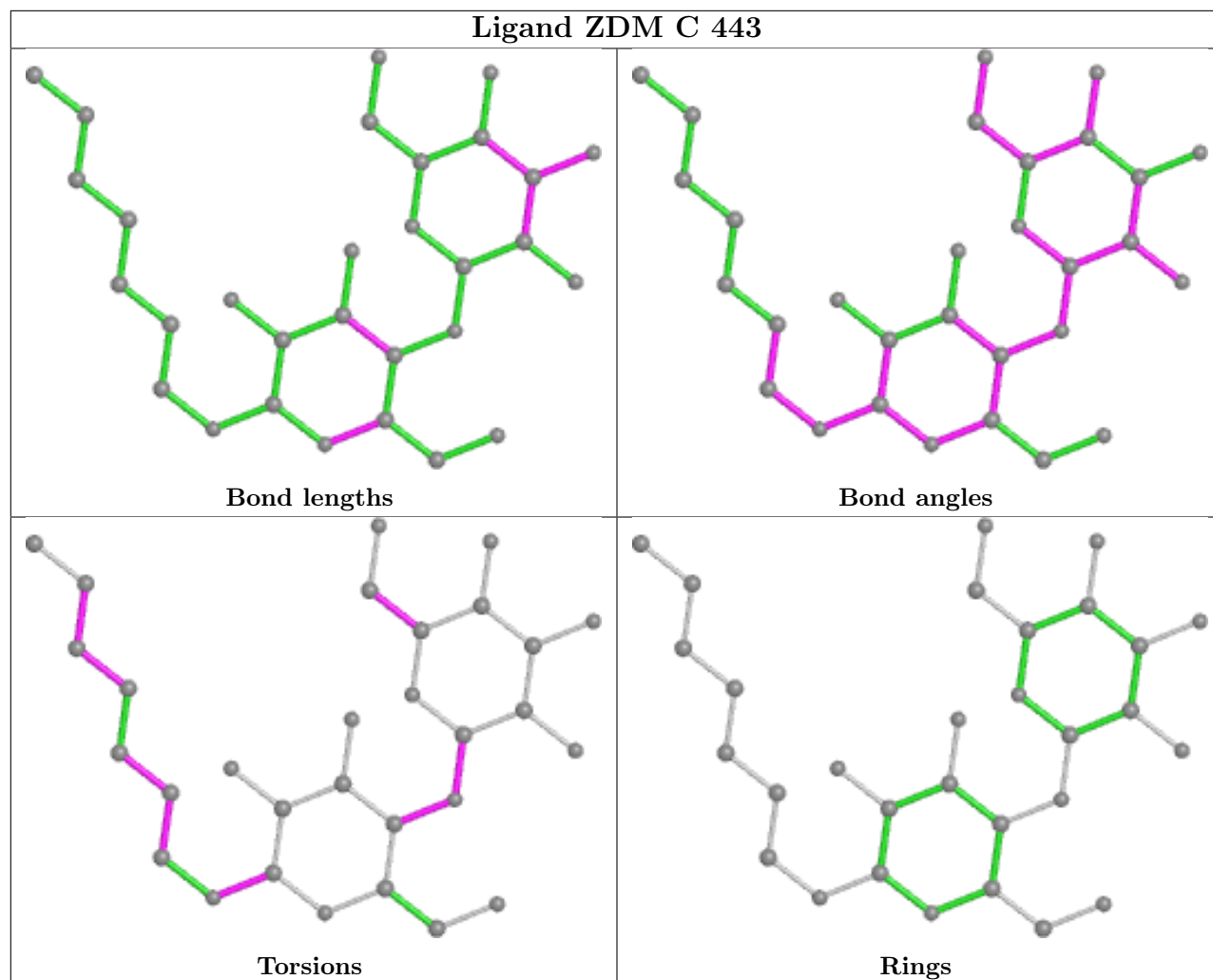
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.









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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	432/442 (97%)	-0.23	8 (1%) 66 65	79, 105, 141, 172	0
1	B	432/442 (97%)	-0.22	6 (1%) 75 75	77, 101, 146, 207	0
1	C	432/442 (97%)	-0.26	4 (0%) 84 84	77, 103, 138, 161	0
1	D	436/442 (98%)	-0.30	6 (1%) 75 75	76, 98, 148, 196	0
All	All	1732/1768 (97%)	-0.25	24 (1%) 75 75	76, 102, 144, 207	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	51	PRO	7.5
1	D	438	ASN	3.9
1	B	54	SER	3.9
1	A	51	PRO	3.8
1	C	313	ARG	3.2
1	C	311	PHE	3.1
1	A	395	GLY	3.1
1	A	323	LEU	3.0
1	B	52	GLY	2.9
1	D	209	PHE	2.9
1	A	368	GLU	2.7
1	D	51	PRO	2.7
1	C	312	ALA	2.6
1	A	274	PHE	2.6
1	D	436	ALA	2.5
1	B	3	ARG	2.4
1	A	340	MET	2.4
1	C	322	ARG	2.3
1	D	437	GLU	2.3
1	D	232	TRP	2.2
1	B	50	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	55	GLU	2.2
1	A	276	ALA	2.2
1	A	343	VAL	2.1

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](#)

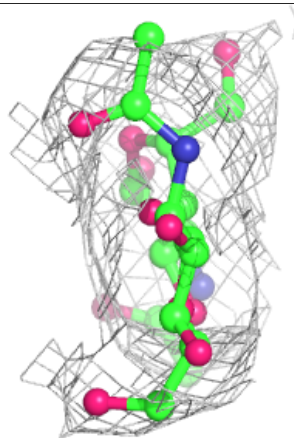
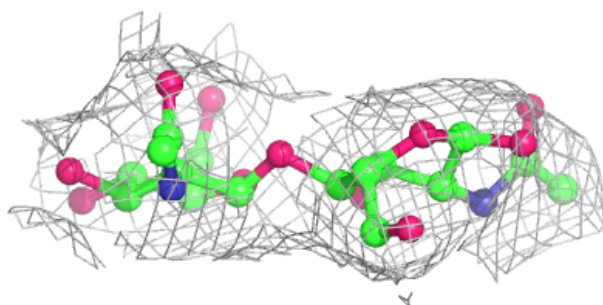
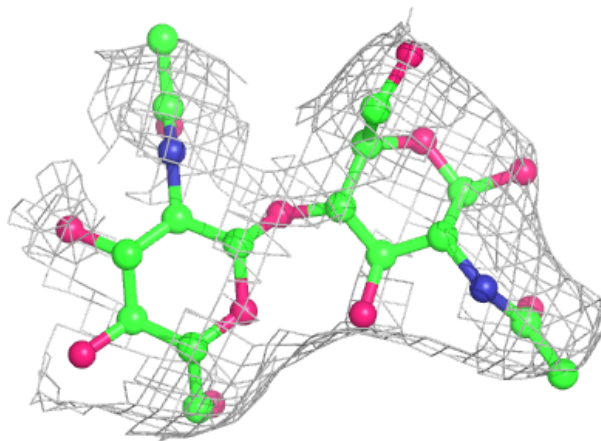
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GLC	F	2	11/12	0.76	0.22	120,131,136,136	0
3	GLC	L	2	11/12	0.83	0.51	115,125,132,134	0
3	GLC	H	2	11/12	0.84	0.37	123,138,141,143	0
3	GLC	F	1	12/12	0.85	0.33	114,133,141,141	0
3	GLC	L	1	12/12	0.88	0.47	116,130,136,136	0
3	GLC	J	1	12/12	0.88	0.23	121,140,148,150	0
3	GLC	H	1	12/12	0.89	0.37	131,136,142,144	0
3	GLC	J	2	11/12	0.90	0.20	119,130,134,135	0
2	NAG	K	1	15/15	0.93	0.22	81,99,103,108	0
2	NAG	E	1	15/15	0.94	0.27	99,105,115,117	0
2	NAG	I	1	15/15	0.95	0.27	101,107,112,116	0
2	NAG	G	1	15/15	0.95	0.25	84,100,106,115	0
2	NAG	E	2	14/15	0.96	0.23	95,103,106,110	0
2	NAG	G	2	14/15	0.96	0.20	88,97,101,106	0
2	NAG	I	2	14/15	0.97	0.20	91,100,107,109	0
2	NAG	K	2	14/15	0.97	0.18	89,95,102,103	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.

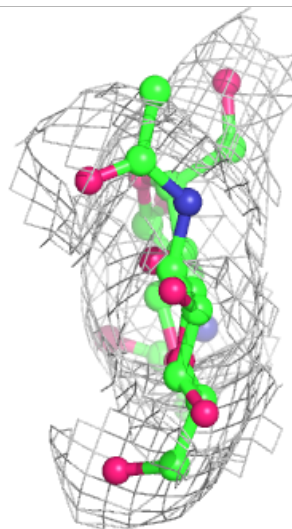
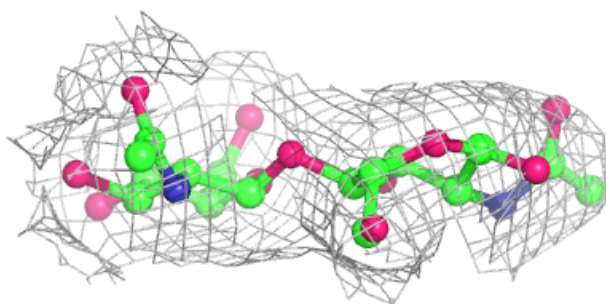
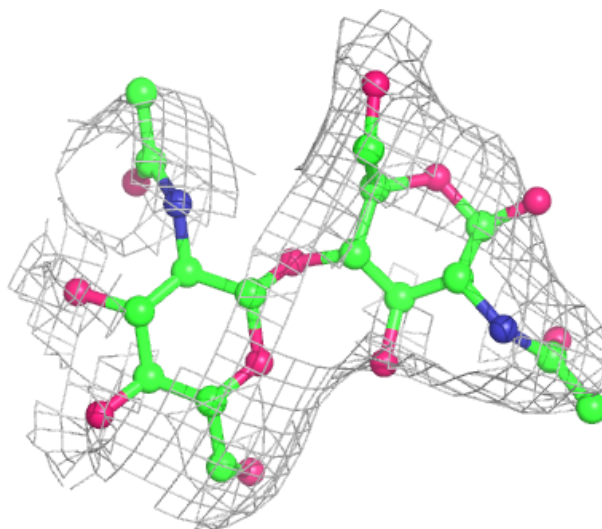
Electron density around Chain E:

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



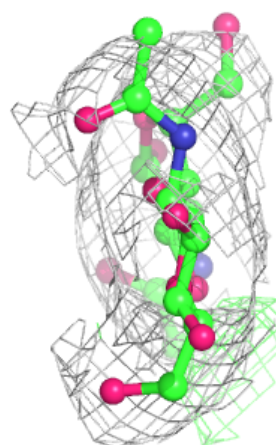
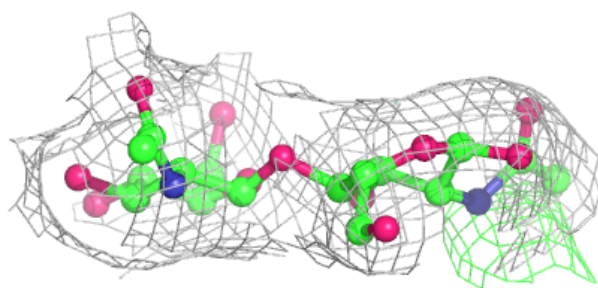
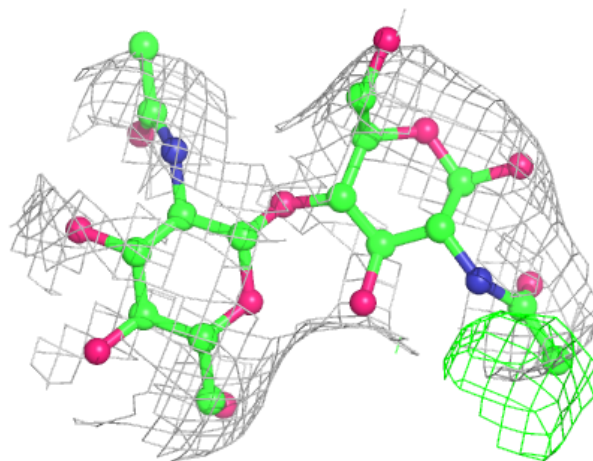
Electron density around Chain G:

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



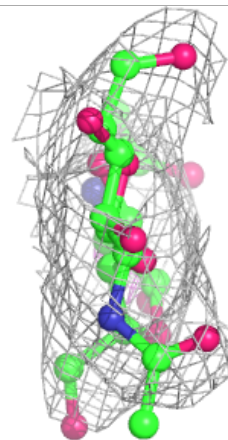
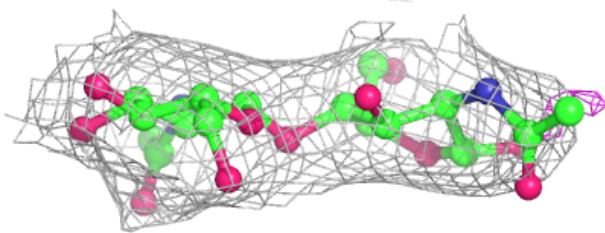
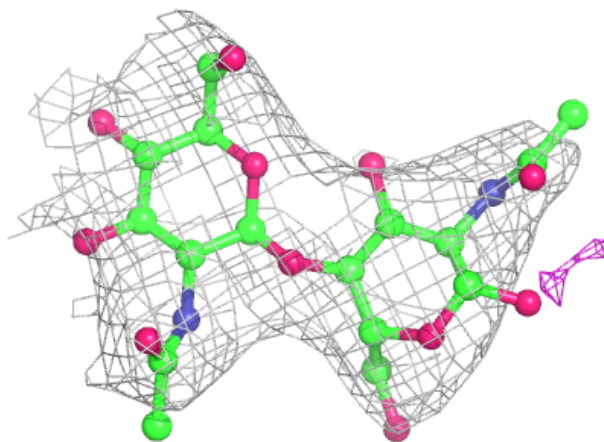
Electron density around Chain I:

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



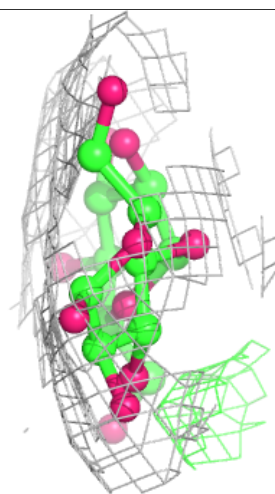
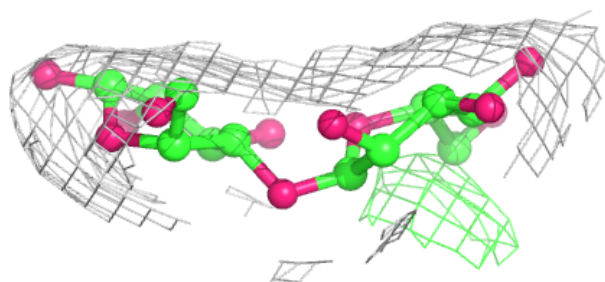
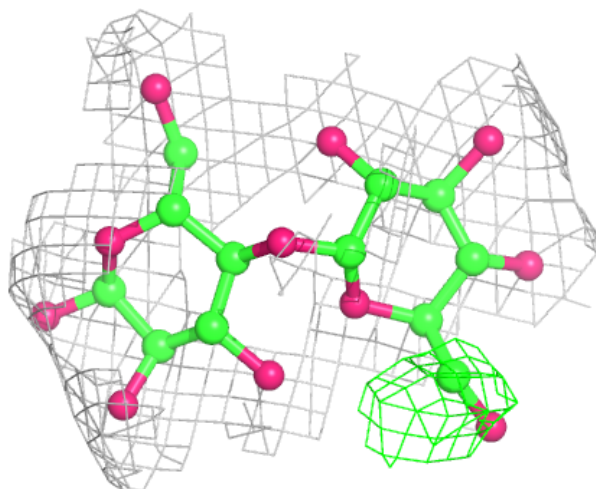
Electron density around Chain K:

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



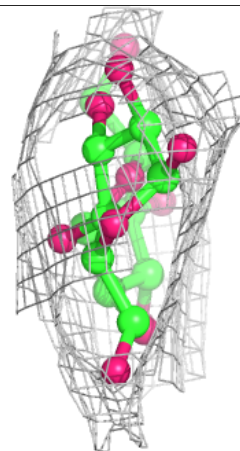
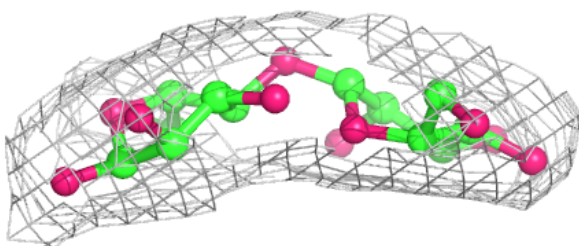
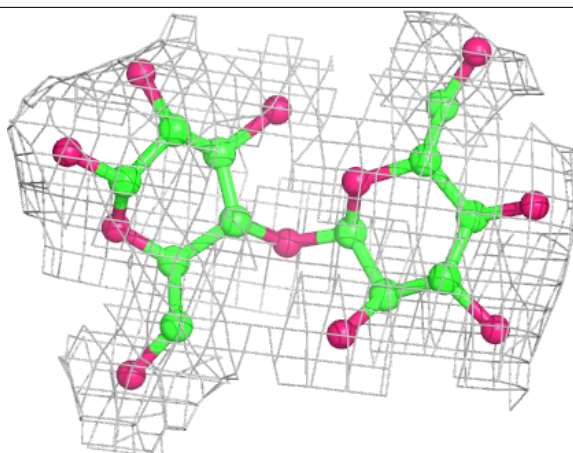
Electron density around Chain F:

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



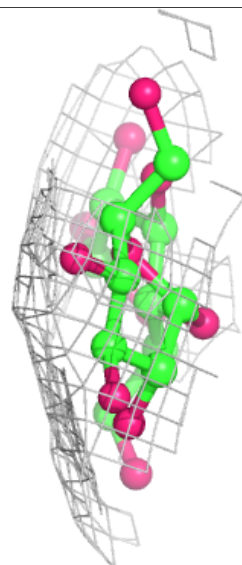
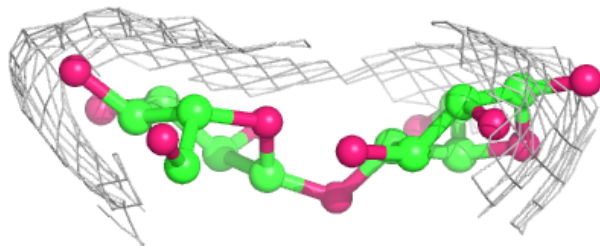
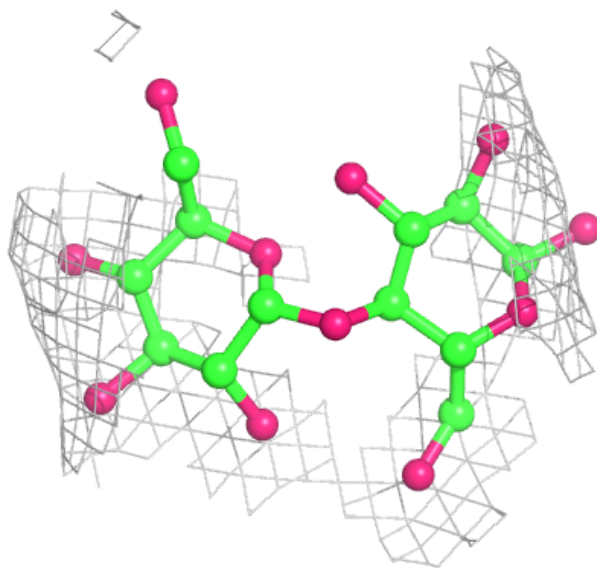
Electron density around Chain H:

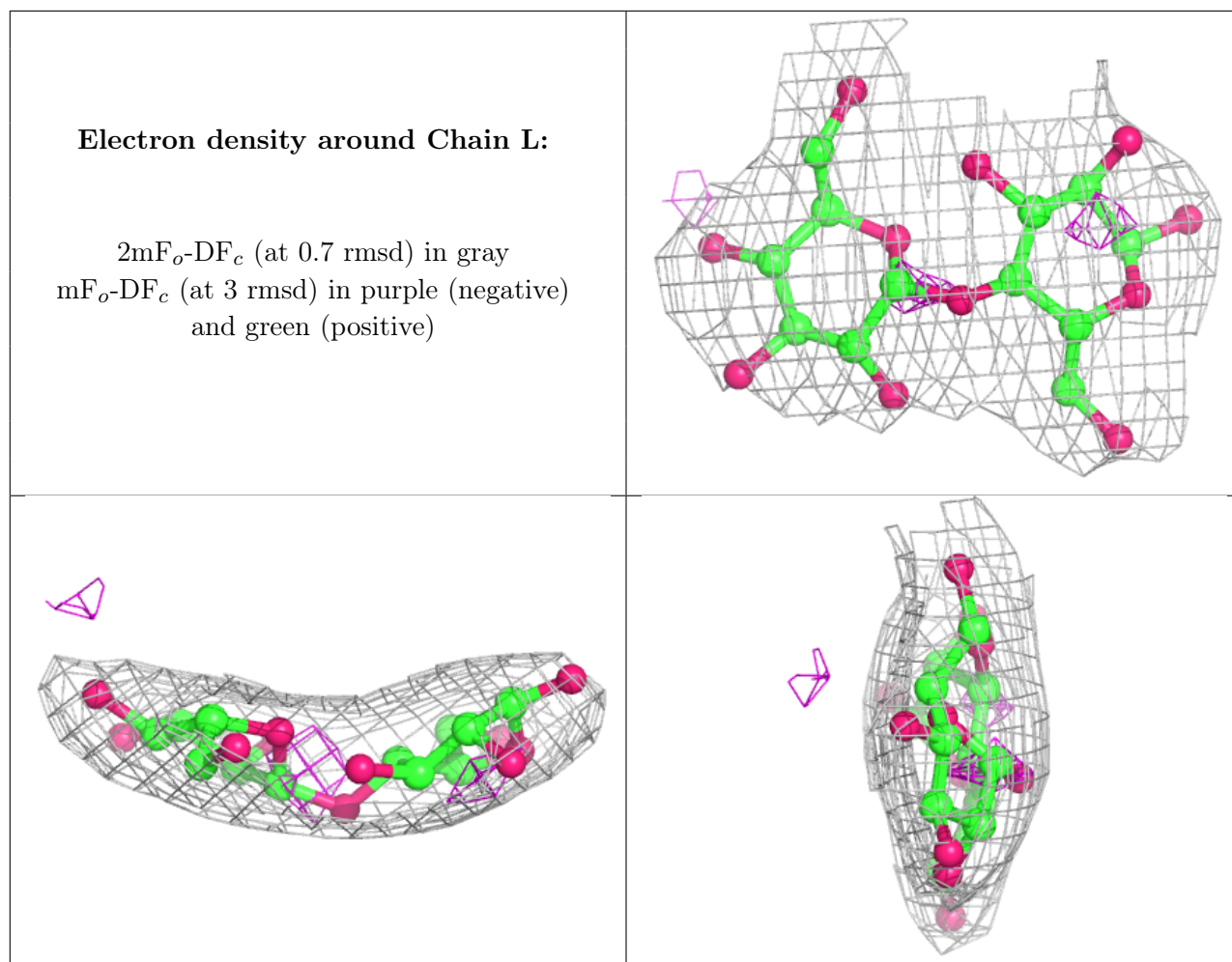
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain J:

$2mF_o-DF_c$ (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.

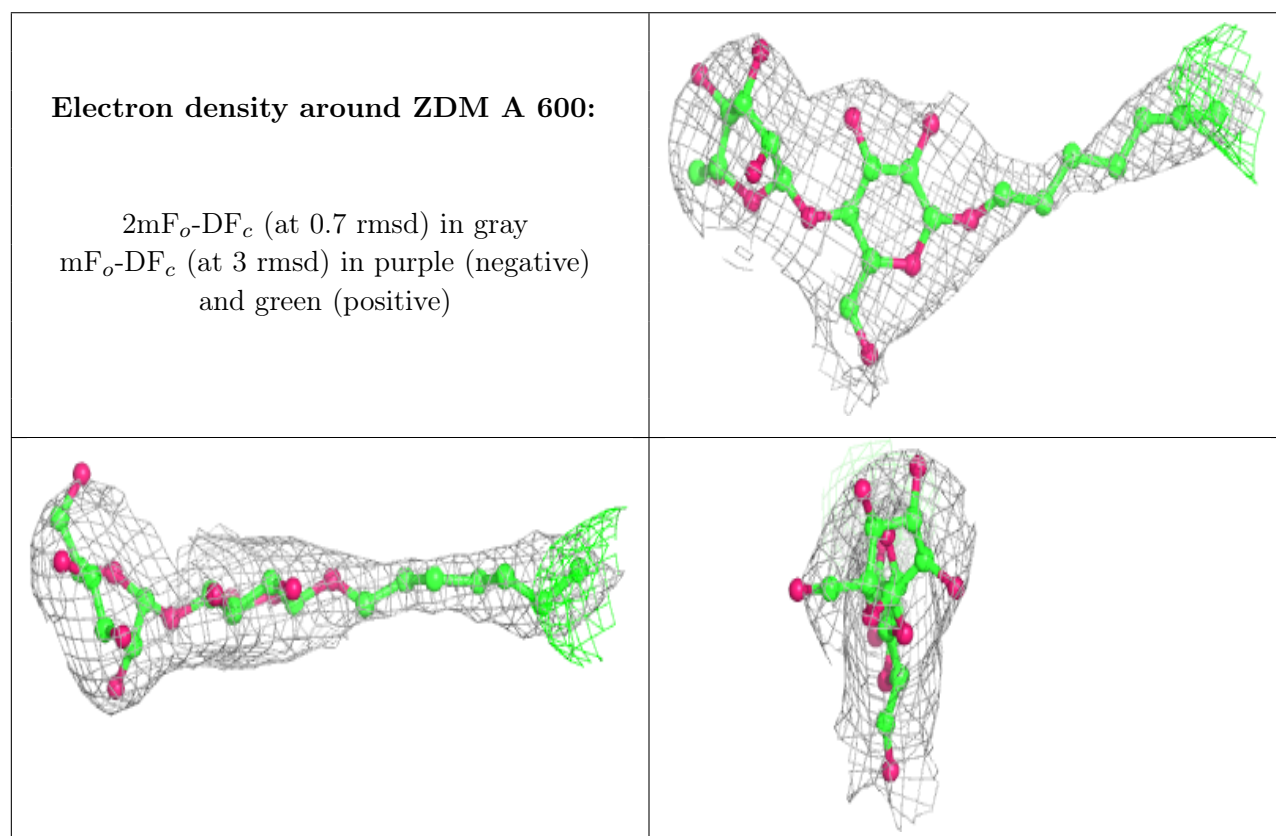
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CIT	C	800	13/13	0.75	0.35	98,116,131,131	0
5	CIT	B	443	13/13	0.81	0.19	120,141,148,148	0
5	CIT	C	445	13/13	0.82	0.21	151,165,175,176	0
5	CIT	B	800	13/13	0.83	0.17	100,114,127,127	0
5	CIT	A	444	13/13	0.84	0.24	84,105,124,128	0
5	CIT	D	800	13/13	0.87	0.16	120,131,139,140	0
4	ZDM	A	600	30/32	0.89	0.23	77,92,107,114	0
5	CIT	C	444	13/13	0.91	0.16	95,117,125,128	0
4	ZDM	C	443	30/32	0.92	0.23	63,89,101,107	0
4	ZDM	A	443	30/32	0.92	0.20	67,90,99,106	0

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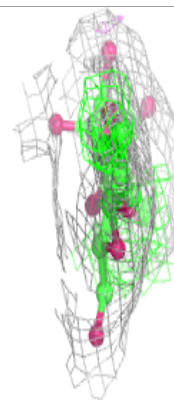
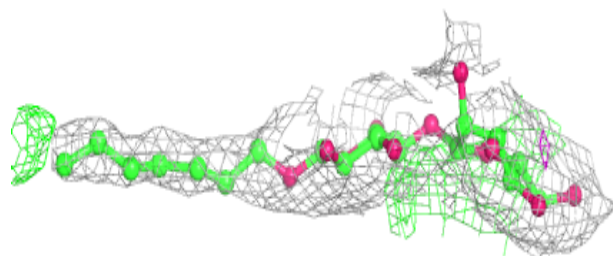
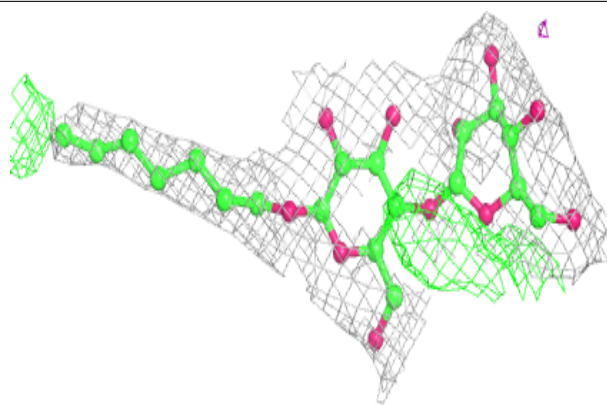
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ZDM	C	600	30/32	0.93	0.23	72,88,100,105	0

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.

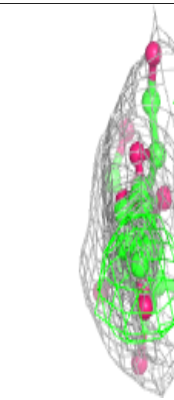
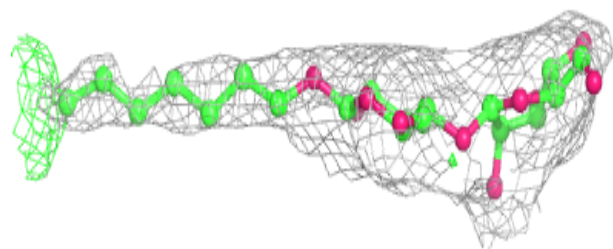
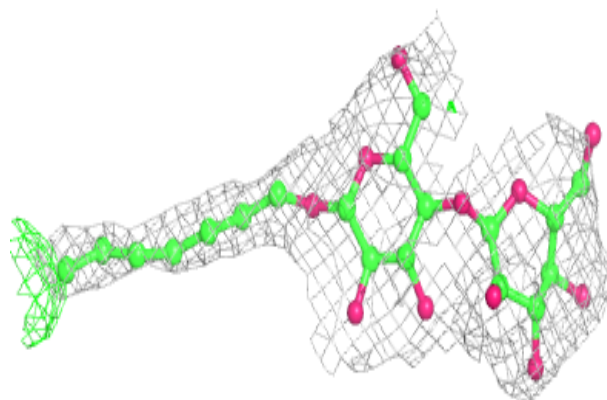


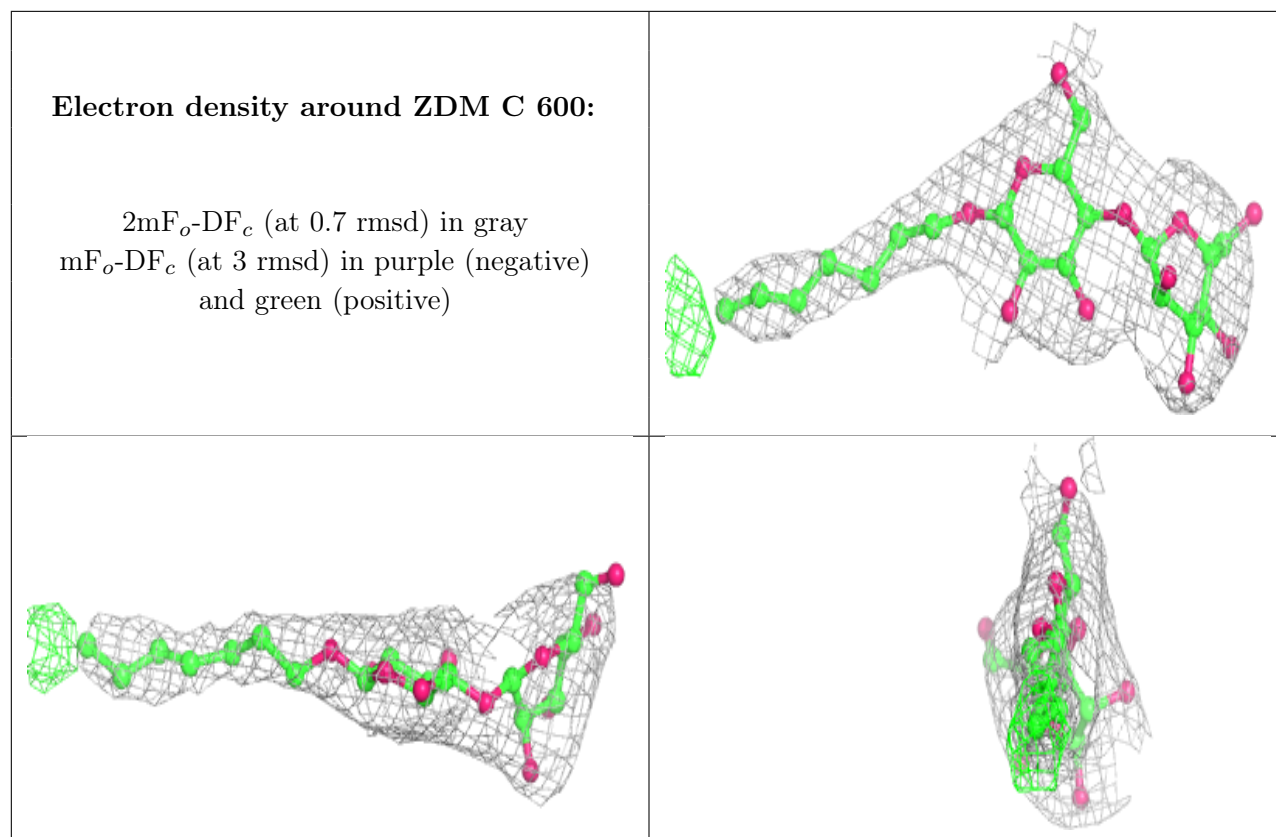
Electron density around ZDM C 443:

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

**Electron density around ZDM A 443:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.