Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 02:43 PM JST

PDB ID	:	7Y4Q
Title	:	Semaphorin 6D in complex with Plexin A1
Authors	:	Tanaka, T.; Neyazaki, M.; Nogi, T.
Deposited on	:	2022-06-16
Resolution	:	4.70 Å(reported)

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 4.70 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.
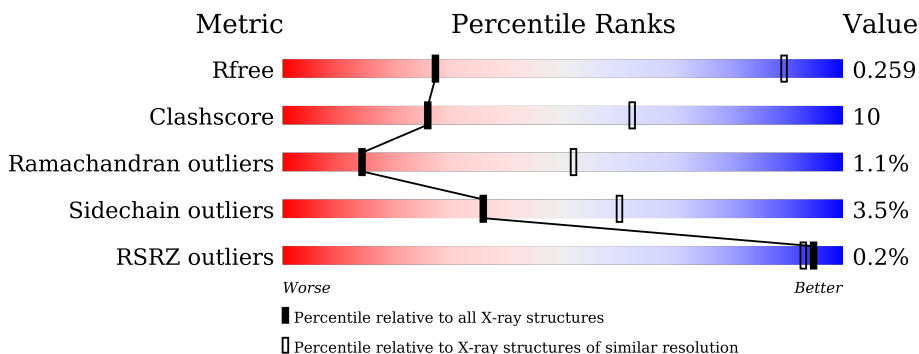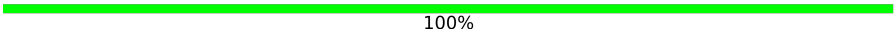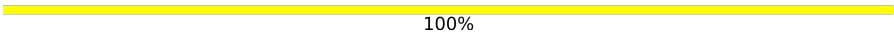

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1085 (5.58-3.80)
Clashscore	141614	1159 (5.60-3.80)
Ramachandran outliers	138981	1094 (5.58-3.80)
Sidechain outliers	138945	1074 (5.58-3.80)
RSRZ outliers	127900	1118 (5.70-3.70)

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

Mol	Chain	Length	Quality of chain
1	A	694	69% 　 24% 　 · ·
1	B	694	71% 　 23% 　 · ·
2	C	552	68% 　 26% 　 · 5%
2	D	552	71% 　 24% 　 · 5%
3	E	2	50% 　 50%
3	F	2	50% 　 50%

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Mol	Chain	Length	Quality of chain
3	G	2	50% 50%
3	H	2	100%
3	I	2	100%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 19075 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 Plexin-A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	670	5235	3304	906	992	33	0	0	0
1	A	670	Total	C	N	O	S	0	0	0
			5235	3304	906	992	33			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	25	GLY	-	expression tag	UNP Q9UIW2
B	26	ARG	-	expression tag	UNP Q9UIW2
B	709	SER	-	expression tag	UNP Q9UIW2
B	710	ARG	-	expression tag	UNP Q9UIW2
B	711	LEU	-	expression tag	UNP Q9UIW2
B	712	GLU	-	expression tag	UNP Q9UIW2
B	713	ASN	-	expression tag	UNP Q9UIW2
B	714	LEU	-	expression tag	UNP Q9UIW2
B	715	TYR	-	expression tag	UNP Q9UIW2
B	716	PHE	-	expression tag	UNP Q9UIW2
B	717	GLN	-	expression tag	UNP Q9UIW2
B	718	GLY	-	expression tag	UNP Q9UIW2
A	25	GLY	-	expression tag	UNP Q9UIW2
A	26	ARG	-	expression tag	UNP Q9UIW2
A	709	SER	-	expression tag	UNP Q9UIW2
A	710	ARG	-	expression tag	UNP Q9UIW2
A	711	LEU	-	expression tag	UNP Q9UIW2
A	712	GLU	-	expression tag	UNP Q9UIW2
A	713	ASN	-	expression tag	UNP Q9UIW2
A	714	LEU	-	expression tag	UNP Q9UIW2
A	715	TYR	-	expression tag	UNP Q9UIW2
A	716	PHE	-	expression tag	UNP Q9UIW2
A	717	GLN	-	expression tag	UNP Q9UIW2
A	718	GLY	-	expression tag	UNP Q9UIW2

- Molecule 2 is a protein called Semaphorin 6D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	527	Total 4213	C 2673	N 730	O 784	S 26	0	0	0
2	C	525	Total 4196	C 2664	N 725	O 781	S 26	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	19	SER	-	expression tag	UNP A0A0G2JZC4
D	20	SER	-	expression tag	UNP A0A0G2JZC4
D	21	ARG	-	expression tag	UNP A0A0G2JZC4
D	332	GLY	SER	engineered mutation	UNP A0A0G2JZC4
C	19	SER	-	expression tag	UNP A0A0G2JZC4
C	20	SER	-	expression tag	UNP A0A0G2JZC4
C	21	ARG	-	expression tag	UNP A0A0G2JZC4
C	332	GLY	SER	engineered mutation	UNP A0A0G2JZC4

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a
cetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total 28	C 16	N 2	O 10	0	0	0
3	H	2	Total 28	C 16	N 2	O 10	0	0	0
3	E	2	Total 28	C 16	N 2	O 10	0	0	0
3	G	2	Total 28	C 16	N 2	O 10	0	0	0
3	I	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).

NAG

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
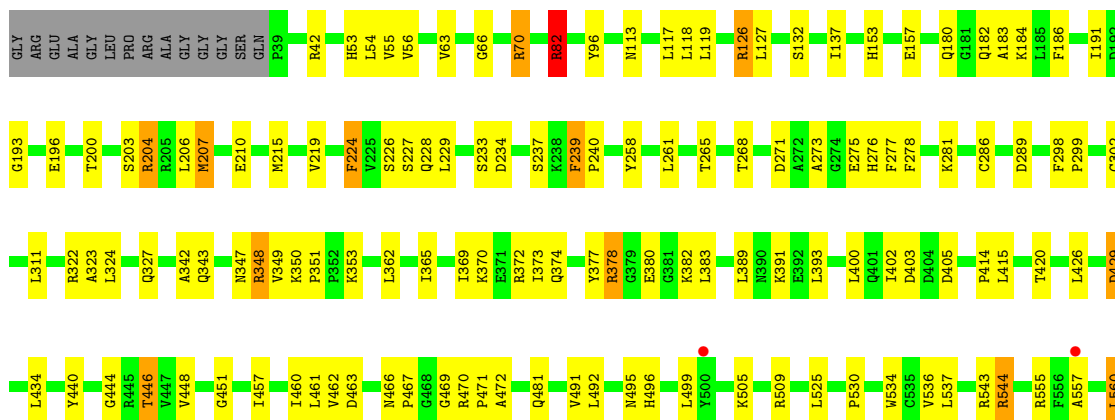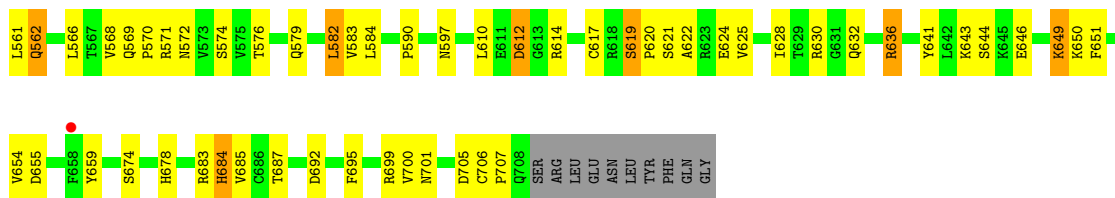
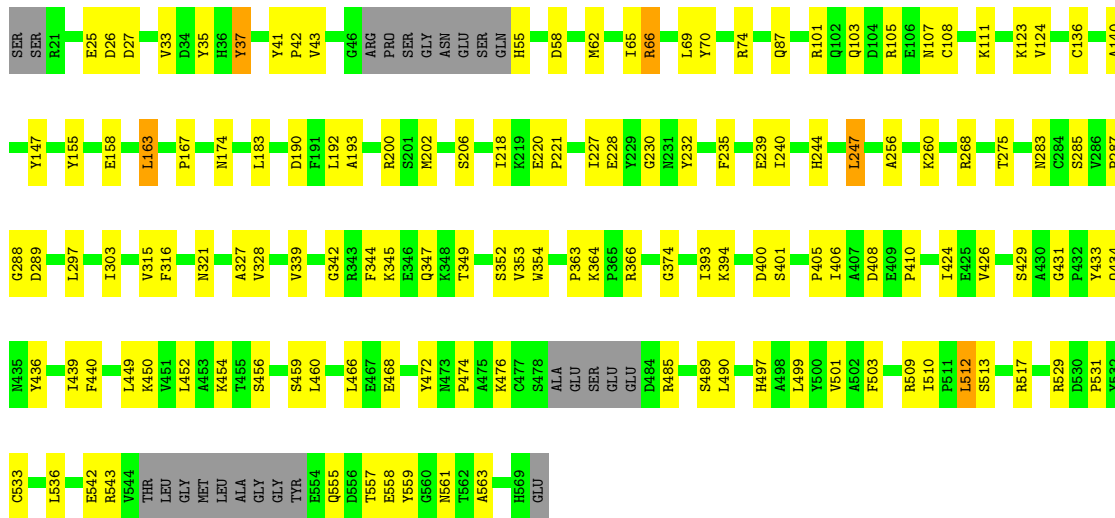- Molecule 1: Plexin-A1

Chain B:

- Molecule 1: Plexin-A1

Chain A:

L561 Q562 L566 T567 V568 Q569 P570 R571 N572 V573 S574 V575 T576 Q579 L582 V583 L584 P590 N597 L610 E611 D612 G613 R614 C617 R618 S619 P620 S621 A622 R623 E624 V625 I628 T629 R630 Q631 Q632 R636 Y641 L642 K643 S644 K645 E646 K649 K650 F651

V654 D655 F658 Y659 S674 H678 H684 V685 C686 T687 D692 F695 R699 V700 N701 D705 C706 P707 Q708 SER ARG LEU GLU ASN LEU TYR PHE GLN GLY

• Molecule 2: Semaphorin 6D

Chain D:

71% 24% • 5%

SER SER R21 E25 D26 D27 V33 D34 Y35 H36 Y37 Y41 P42 V43 G46 ARG PRO SER GLY ASN GLU SER GLN H55 D58 M62 I65 R66 L69 Y70 R74 Q87 R101 Q102 Q103 D104 R105 E106 N107 C108 K111 K123 V124 C136 A140

Y147 Y155 E158 L163 P167 N174 L183 D190 F191 L192 A193 R200 S201 M202 S206 I218 K219 E220 P221 I227 E228 Y229 G230 N231 Y232 F235 E239 I240 H244 L247 A256 K260 R268 T275 N283 C284 S285 V286 P287

G288 D289 L297 I303 V315 F316 N321 A327 V328 V339 G342 R343 F344 K345 E346 Q347 K348 T349 S352 V353 W354 P363 K364 P365 R366 G374 I393 K394 D400 S401 P405 I406 A407 D408 E409 P410 I424 E425 V426 S429 A430 G431 P432 Y433 Q434

N435 Y436 I439 F440 L449 K450 V451 L452 A453 K454 T455 S456 S459 L460 L466 E467 E468 Y472 N473 P474 A475 K476 C477 S478 ALA GLU SER GLU GLU D484 R485 S489 L490 H497 A498 L499 V500 V501 A502 F503 R509 I510 P511 L512 S513 R517 R529 D530 P531 Y532

C533 L536 E542 R543 V544 THR LEU GLY MET LEU ALA GLY GLY TYR E554 Q555 D556 T557 E558 Y559 G560 N561 T562 A563 H569 GLU

• Molecule 2: Semaphorin 6D

Chain C:

68% 26% • 5%

SER SER ARG SER F23 D26 L30 Y35 H36 Y37 P42 V43 F44 R45 G46 ARG PRO SER GLY ASN GLU SER GLN H55 R56 M62 I65 L69 Y70 R74 D75 Q76 V77 Y78 Q87 K94 K95 L96 R101 D104 R105 E106 N107 K111 F121

V124 P127 V133 C136 R146 Y147 Y148 L153 E154 Y155 L163 A164 R165 V188 A189 D190 F191 L192 A193 Y199 R200 S201 M202 R209 T210 S215 K216 W217 I218 K219 E220 P221 H222 F223 A226 I227 E228 Y234 F237 A241 V242 E243 H244 N245 N246 L247

G248 K249 A250 V251 Y252 A256 R257 K260 R268 K279 A280 R281 L282 N283 C284 S285 V286 P287 F291 S299 I300 T301 D302 N307 V312 I313 G314 V315 Q319 L320 N321 V328 V339 F340 K341 F344 K345 V353 P358 K361 V362 P363 K364 P365 R366

Y379 K380 T381 S382 I383 D387 D400 V403 D408 T413 R416 V417 R418 I424 E425 V426 D427 R428 S429 A430 G431 P432 Y433 Q434 I439 F440 K450 V451 L452 S456 L460 N461 D462 L466 Y472 N473 P474 S478 ALA GLU SER GLU GLU D484

L490 Q491 L492 H497 A498 L499 Y500 V508 R509 L512 S513 R514 C515 E516 R517 Y518 G519 C525 I526 R529 D530 P531 Y532 C533 G534 W535 G539 V540 R543 V544 THR LEU GLY MET LEU ALA GLY GLY TYR E554 Q555 D567 C568 H569 GLU

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

Chain F:

50% 50%

NAG1
NAG2

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

Chain H: 100%

NAG1
NAG2

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

Chain E: 50% 50%

NAG1
NAG2

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

Chain G: 50% 50%

NAG1
NAG2

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

Chain I: 100%

NAG1
NAG2

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	173.14Å 198.51Å 180.50Å 90.00° 117.83° 90.00°	Depositor
Resolution (Å)	49.43 – 4.70 49.43 – 4.70	Depositor EDS
% Data completeness (in resolution range)	95.1 (49.43-4.70) 93.3 (49.43-4.70)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 4.64Å)	Xtriage
Refinement program	PHENIX 1.13_2998+SVN	Depositor
R, R_{free}	0.241 , 0.258 0.239 , 0.259	Depositor DCC
R_{free} test set	2523 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å^2)	157.7	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 110.6	EDS
L-test for twinning[2]	$< |L| > = 0.39, < L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.059 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	19075	wwPDB-VP
Average B, all atoms (Å^2)	200.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.37	0/5357	0.75	8/7272 (0.1%)
1	B	0.34	0/5357	0.72	4/7272 (0.1%)
2	C	0.35	0/4298	0.67	0/5821
2	D	0.34	0/4315	0.71	3/5843 (0.1%)
All	All	0.35	0/19327	0.72	15/26208 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	2
All	All	0	6

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	82	ARG	NE-CZ-NH2	-11.83	114.39	120.30
1	A	82	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	B	80	LEU	CA-CB-CG	8.46	134.77	115.30
1	A	353	LYS	CD-CE-NZ	-7.91	93.50	111.70
2	D	66	ARG	NE-CZ-NH2	7.89	124.25	120.30
2	D	66	ARG	NE-CZ-NH1	-7.86	116.37	120.30
1	B	543	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	A	70	ARG	CG-CD-NE	-5.89	99.42	111.80
1	A	572	ASN	N-CA-CB	-5.65	100.42	110.60
1	A	560	LEU	CA-CB-CG	5.60	128.18	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	469	GLY	C-N-CA	5.49	135.44	121.70
1	B	207	MET	CA-CB-CG	5.20	122.14	113.30
1	A	224	PHE	CB-CG-CD2	-5.11	117.22	120.80
2	D	559	TYR	CB-CG-CD1	-5.04	117.98	121.00
1	B	108	LEU	CA-CB-CG	5.01	126.81	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	ARG	Mainchain
1	A	525	LEU	Mainchain
1	A	571	ARG	Mainchain
1	A	82	ARG	Mainchain
1	B	651	PHE	Mainchain
1	B	82	ARG	Mainchain

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	5235	0	5084	120	0
1	B	5235	0	5085	108	0
2	C	4196	0	4075	99	0
2	D	4213	0	4093	84	0
3	E	28	0	25	1	0
3	F	28	0	25	0	0
3	G	28	0	25	1	0
3	H	28	0	25	0	0
3	I	28	0	25	2	0
4	A	28	0	26	2	0
4	B	28	0	26	2	0
All	All	19075	0	18514	394	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 10.

All (394) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:GLN:HG2	1:A:636:ARG:HB2	1.52	0.92
1:A:393:LEU:HD21	2:C:192:LEU:HD22	1.58	0.85
1:B:239:PHE:HZ	1:B:265:THR:HG22	1.43	0.83
2:D:123:LYS:HB3	2:D:174:ASN:HD21	1.43	0.83
2:D:58:ASP:HB2	2:D:74:ARG:HB2	1.60	0.83
2:D:43:VAL:HG21	2:D:476:LYS:HG2	1.62	0.81
2:C:165:ARG:HH21	2:C:201:SER:HB3	1.43	0.79
1:A:224:PHE:HE1	2:C:164:ALA:HB2	1.49	0.78
1:B:239:PHE:CZ	1:B:265:THR:HG22	2.21	0.75
2:D:218:ILE:HG12	2:D:221:PRO:HG3	1.66	0.75
2:D:426:VAL:HG22	2:D:439:ILE:HG12	1.68	0.74
2:D:490:LEU:HD13	2:D:499:LEU:HD21	1.69	0.74
1:A:324:LEU:HB2	1:A:446:THR:HG21	1.68	0.73
2:D:429:SER:HB2	2:D:434:GLN:HB3	1.70	0.73
2:D:321:ASN:ND2	2:C:287:PRO:O	2.21	0.73
2:D:529:ARG:NH2	2:D:558:GLU:O	2.23	0.72
1:A:426:LEU:HA	1:A:471:PRO:HG2	1.71	0.72
1:B:327:GLN:NE2	1:B:463:ASP:OD1	2.22	0.70
1:A:268:THR:HG22	1:A:277:PHE:H	1.58	0.69
2:C:345:LYS:HE2	2:C:400:ASP:HA	1.72	0.69
2:C:513:SER:OG	2:C:515:CYS:SG	2.44	0.69
2:D:103:GLN:O	2:D:107:ASN:ND2	2.26	0.69
1:A:56:VAL:HG22	1:A:63:VAL:HG22	1.73	0.69
1:A:700:VAL:HG13	1:A:705:ASP:HB2	1.76	0.67
2:C:500:TYR:CE2	2:C:509:ARG:HG3	2.30	0.67
1:B:324:LEU:HG	1:B:446:THR:HG21	1.76	0.67
1:A:389:LEU:HD21	1:A:414:PRO:HD2	1.75	0.67
1:B:370:LYS:O	1:B:374:GLN:HB2	1.95	0.67
1:B:459:LYS:NZ	1:B:512:VAL:O	2.29	0.66
1:A:706:CYS:HB3	1:A:707:PRO:HD2	1.78	0.65
2:D:33:VAL:HG13	2:D:37:TYR:HB3	1.79	0.65
1:A:649:LYS:HD2	1:A:650:LYS:H	1.61	0.65
2:D:124:VAL:HB	2:D:136:CYS:HB2	1.78	0.65
1:A:239:PHE:CZ	1:A:265:THR:HG22	2.32	0.65
1:B:155:ARG:HB2	1:B:158:HIS:CD2	2.32	0.64
2:C:513:SER:OG	2:C:533:CYS:SG	2.55	0.64
2:C:431:GLY:HA2	2:C:531:PRO:HB2	1.80	0.64
2:D:287:PRO:O	2:C:321:ASN:ND2	2.29	0.63
1:B:566:LEU:HB3	1:B:654:VAL:HB	1.81	0.63
2:D:147:TYR:HE2	2:D:202:MET:HE1	1.64	0.62
1:A:446:THR:HG23	1:A:462:VAL:HG23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:217:TRP:O	2:C:279:LYS:NZ	2.29	0.62
2:C:42:PRO:HG2	2:C:509:ARG:HB3	1.80	0.62
1:A:347:ASN:O	1:A:349:VAL:N	2.31	0.62
1:A:649:LYS:HD2	1:A:650:LYS:N	2.15	0.62
2:D:433:TYR:CD2	3:E:1:NAG:H62	2.35	0.61
1:A:426:LEU:HD13	1:A:462:VAL:HG11	1.83	0.61
1:A:203:SER:HB3	1:A:227:SER:HB2	1.80	0.61
1:A:118:LEU:HD11	1:A:127:LEU:HD21	1.80	0.61
1:B:373:ILE:HG22	1:B:415:LEU:HD23	1.83	0.61
2:C:65:ILE:HD12	2:C:70:TYR:HE2	1.66	0.61
1:A:323:ALA:O	1:A:327:GLN:HG3	2.01	0.61
1:B:466:ASN:O	1:B:468:GLY:N	2.30	0.60
2:D:35:TYR:CE1	2:D:474:PRO:HD2	2.35	0.60
2:D:454:LYS:HE3	2:D:460:LEU:O	2.01	0.60
1:B:411:PHE:HA	2:D:192:LEU:HD21	1.82	0.60
1:A:461:LEU:HD22	1:A:530:PRO:HG3	1.84	0.60
1:B:582:LEU:HD13	1:B:584:LEU:HD13	1.83	0.60
1:B:286:CYS:HB2	1:B:289:ASP:HB2	1.84	0.60
2:C:344:PHE:HE1	2:C:366:ARG:NH1	1.99	0.60
2:D:244:HIS:CE1	2:D:247:LEU:HD21	2.37	0.60
2:C:268:ARG:NE	2:C:387:ASP:OD2	2.34	0.60
1:B:196:GLU:OE2	2:D:394:LYS:NZ	2.32	0.59
1:B:700:VAL:HG13	1:B:705:ASP:HB2	1.84	0.59
2:C:315:VAL:HG22	2:C:328:VAL:HG22	1.83	0.59
2:D:342:GLY:O	2:D:366:ARG:NH2	2.34	0.59
1:A:373:ILE:HG22	1:A:415:LEU:HD23	1.84	0.58
1:A:184:LYS:HD3	1:A:219:VAL:HG21	1.84	0.58
1:B:268:THR:HG22	1:B:277:PHE:H	1.68	0.58
2:C:228:GLU:HG3	2:C:260:LYS:HE2	1.86	0.58
1:B:451:GLY:HA2	1:B:457:ILE:HD13	1.86	0.58
2:D:62:MET:HB2	2:D:69:LEU:HD11	1.85	0.58
2:C:96:LEU:HD12	2:C:153:LEU:HB3	1.86	0.58
1:B:298:PHE:HZ	1:B:372:ARG:HB2	1.69	0.57
1:A:370:LYS:O	1:A:374:GLN:HB2	2.05	0.57
1:B:582:LEU:HD11	1:B:617:CYS:SG	2.45	0.57
1:A:537:LEU:HD21	1:A:646:GLU:HB3	1.87	0.57
2:D:339:VAL:HG13	2:D:401:SER:HB2	1.87	0.57
2:C:365:PRO:HG3	2:C:379:TYR:CE2	2.40	0.57
1:A:224:PHE:CD1	2:C:163:LEU:HD23	2.40	0.57
1:A:348:ARG:O	1:A:351:PRO:HD3	2.04	0.57
2:C:440:PHE:CE1	2:C:450:LYS:HG3	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:LEU:HG	1:B:185:LEU:HD13	1.86	0.56
1:A:566:LEU:HB3	1:A:654:VAL:HB	1.87	0.56
1:A:687:THR:HG21	1:A:692:ASP:HB2	1.86	0.56
1:A:96:TYR:O	2:C:268:ARG:HG2	2.05	0.56
2:C:146:ARG:HD3	2:C:155:TYR:CD1	2.41	0.56
1:A:641:TYR:CD2	1:A:650:LYS:HD2	2.40	0.56
1:B:281:LYS:HD3	1:B:299:PRO:HG3	1.86	0.56
1:A:281:LYS:HD3	1:A:299:PRO:HG3	1.88	0.56
1:A:536:VAL:HG21	1:A:590:PRO:HD3	1.88	0.56
2:C:433:TYR:CG	3:I:1:NAG:H62	2.40	0.56
1:B:411:PHE:CE1	2:D:111:LYS:HA	2.40	0.56
2:D:285:SER:O	2:D:410:PRO:HD3	2.06	0.56
1:A:429:ASP:OD1	1:A:434:LEU:HG	2.05	0.56
1:A:597:ASN:HB2	1:A:643:LYS:HB3	1.88	0.56
2:C:190:ASP:OD1	2:C:193:ALA:N	2.38	0.55
2:C:429:SER:HB2	2:C:434:GLN:HB3	1.87	0.55
2:C:65:ILE:HD12	2:C:70:TYR:CE2	2.41	0.55
2:C:241:ALA:HB2	2:C:252:TYR:HB2	1.87	0.55
2:D:497:HIS:CE1	2:D:512:LEU:HB2	2.42	0.55
1:A:226:SER:O	1:A:228:GLN:N	2.38	0.55
2:C:215:SER:HB2	2:C:219:LYS:HD2	1.89	0.55
2:C:339:VAL:HG21	2:C:403:VAL:HG22	1.88	0.55
1:B:42:ARG:HB2	1:B:509:ARG:HB3	1.89	0.55
2:C:127:PRO:HA	2:C:133:VAL:HA	1.89	0.55
1:B:140:PHE:HE1	1:B:216:PHE:CZ	2.25	0.55
1:A:462:VAL:HG12	1:A:472:ALA:HB2	1.88	0.55
2:D:25:GLU:HG2	2:D:26:ASP:H	1.72	0.55
1:B:470:ARG:HH21	1:B:470:ARG:HB2	1.73	0.54
2:D:531:PRO:HA	2:D:557:THR:HG21	1.90	0.54
1:B:239:PHE:HD1	1:B:242:PHE:HB2	1.73	0.54
1:B:383:LEU:HD23	1:B:383:LEU:H	1.72	0.54
1:A:186:PHE:O	1:A:258:TYR:OH	2.26	0.54
1:A:683:ARG:HG2	1:A:685:VAL:HG13	1.90	0.54
2:D:227:ILE:HG21	2:D:303:ILE:HG13	1.90	0.54
2:C:44:PHE:HZ	2:C:78:TYR:CG	2.25	0.54
2:C:513:SER:O	2:C:543:ARG:NH2	2.41	0.53
1:B:513:GLU:HG2	1:B:515:CYS:SG	2.49	0.53
1:A:405:ASP:OD1	1:A:405:ASP:N	2.42	0.53
2:C:246:ASN:O	2:C:247:LEU:HG	2.08	0.53
1:A:699:ARG:HD2	1:A:699:ARG:O	2.08	0.53
2:C:526:ILE:HD11	2:C:535:TRP:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:123:LYS:HB3	2:D:174:ASN:ND2	2.19	0.53
2:C:452:LEU:HB2	2:C:466:LEU:HD11	1.91	0.53
2:D:449:LEU:HD23	2:D:468:GLU:HG3	1.90	0.53
1:A:239:PHE:HZ	1:A:265:THR:HG22	1.73	0.53
2:C:440:PHE:HE1	2:C:450:LYS:HG3	1.73	0.53
2:C:472:TYR:O	2:C:474:PRO:HD3	2.09	0.53
2:C:490:LEU:HD13	2:C:499:LEU:HD21	1.91	0.53
1:B:585:GLN:HG3	1:B:614:ARG:HG3	1.91	0.52
1:B:640:LEU:HB3	1:B:654:VAL:HG13	1.91	0.52
2:D:283:ASN:O	2:D:405:PRO:HD3	2.09	0.52
1:B:671:VAL:HG11	1:B:703:SER:N	2.25	0.52
1:A:362:LEU:HA	1:A:365:ILE:HD12	1.92	0.52
1:A:568:VAL:HG22	1:A:584:LEU:HG	1.90	0.52
2:C:381:THR:HG23	2:C:383:ILE:H	1.74	0.52
2:C:433:TYR:CD2	3:I:1:NAG:H62	2.45	0.52
2:C:492:LEU:HA	2:C:499:LEU:HD12	1.92	0.52
1:B:234:ASP:O	1:B:237:SER:HB3	2.09	0.52
1:B:362:LEU:HA	1:B:365:ILE:HD12	1.91	0.52
1:B:139:GLN:HG2	1:B:151:GLU:HG3	1.92	0.52
2:D:345:LYS:HB2	2:D:400:ASP:HA	1.91	0.52
1:A:349:VAL:HG13	1:A:350:LYS:HG2	1.91	0.52
2:D:454:LYS:HG3	2:D:459:SER:HB3	1.92	0.52
1:B:378:ARG:HD3	1:B:380:GLU:OE2	2.09	0.51
2:D:561:ASN:C	2:D:563:ALA:H	2.12	0.51
1:B:393:LEU:HD22	2:D:192:LEU:HB3	1.92	0.51
1:A:451:GLY:HA2	1:A:457:ILE:HD13	1.92	0.51
1:B:126:ARG:HH11	1:B:210:GLU:HG3	1.75	0.51
1:B:152:PRO:HB2	1:B:158:HIS:CE1	2.45	0.51
1:A:491:VAL:O	1:A:499:LEU:HD12	2.10	0.51
1:B:231:ILE:HD11	1:B:244:ILE:HD12	1.93	0.51
1:A:299:PRO:HB2	1:A:420:THR:HG22	1.92	0.51
1:B:298:PHE:HZ	1:B:372:ARG:CB	2.24	0.50
1:B:42:ARG:NH1	4:B:1001:NAG:H81	2.26	0.50
1:B:180:GLN:O	1:B:182:GLN:N	2.44	0.50
1:A:377:TYR:HE2	1:A:400:LEU:HD23	1.77	0.50
2:C:251:VAL:H	2:C:319:GLN:NE2	2.08	0.50
1:A:137:ILE:HG21	1:A:153:HIS:HB3	1.93	0.50
2:C:94:LYS:HB3	2:C:153:LEU:HD11	1.93	0.50
1:B:391:LYS:H	1:B:391:LYS:HD2	1.77	0.50
1:A:196:GLU:OE1	1:A:196:GLU:N	2.42	0.50
2:C:533:CYS:O	2:C:555:GLN:NE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:450:LYS:NZ	2:C:512:LEU:O	2.41	0.50
2:D:344:PHE:HE1	2:D:366:ARG:NH1	2.10	0.50
2:C:30:LEU:HD12	2:C:466:LEU:HA	1.93	0.50
2:C:241:ALA:HB2	2:C:252:TYR:CG	2.46	0.50
2:C:514:ARG:HE	2:C:517:ARG:HB2	1.76	0.50
1:B:362:LEU:O	1:B:366:LYS:HG3	2.12	0.50
1:B:374:GLN:HG3	1:B:378:ARG:NH1	2.27	0.50
2:D:315:VAL:HG22	2:D:328:VAL:HG22	1.94	0.50
1:A:544:ARG:O	1:A:544:ARG:HG3	2.12	0.49
1:A:224:PHE:CG	2:C:163:LEU:HD23	2.47	0.49
2:C:35:TYR:CE1	2:C:474:PRO:HD2	2.47	0.49
1:A:117:LEU:HD21	1:A:119:LEU:HD12	1.93	0.49
2:C:256:ALA:HA	2:C:279:LYS:HA	1.94	0.49
1:B:117:LEU:HD21	1:B:119:LEU:HD12	1.94	0.49
1:A:534:TRP:HB3	1:A:557:ALA:HB3	1.95	0.49
1:B:456:ARG:HD3	1:B:477:SER:OG	2.13	0.49
1:A:322:ARG:H	1:A:444:GLY:HA2	1.77	0.49
1:A:674:SER:HB3	4:A:1002:NAG:H82	1.93	0.49
2:D:536:LEU:HD11	2:D:542:GLU:HB2	1.94	0.49
2:D:101:ARG:O	2:D:105:ARG:HG3	2.13	0.49
2:D:497:HIS:HE1	2:D:513:SER:H	1.61	0.49
2:C:199:TYR:CE2	2:C:201:SER:HB2	2.48	0.49
1:B:537:LEU:O	1:B:647:THR:HG21	2.13	0.49
2:C:365:PRO:HG3	2:C:379:TYR:HE2	1.76	0.48
1:B:251:ARG:HG2	1:B:256:VAL:HG12	1.94	0.48
2:C:124:VAL:HB	2:C:136:CYS:HB2	1.95	0.48
1:B:525:LEU:HD11	1:B:557:ALA:O	2.13	0.48
1:B:96:TYR:CE1	1:B:197:TYR:HB3	2.49	0.48
2:D:440:PHE:CE1	2:D:450:LYS:HG3	2.48	0.48
1:B:690:VAL:HG21	1:B:699:ARG:HD2	1.93	0.48
1:A:706:CYS:HB3	1:A:707:PRO:CD	2.44	0.48
2:D:174:ASN:OD1	2:D:174:ASN:N	2.46	0.48
2:C:234:TYR:CD1	2:C:257:ARG:HB2	2.49	0.48
1:B:495:ASN:OD1	1:B:495:ASN:N	2.44	0.48
1:A:273:ALA:HB3	1:A:275:GLU:OE1	2.14	0.48
2:D:472:TYR:HB2	2:D:503:PHE:CE2	2.49	0.48
2:C:364:LYS:HD3	2:C:364:LYS:HA	1.50	0.48
1:A:582:LEU:HD11	1:A:617:CYS:SG	2.53	0.48
2:D:288:GLY:HA3	2:C:321:ASN:ND2	2.29	0.48
2:C:43:VAL:HG22	2:C:508:VAL:HG22	1.96	0.48
1:B:96:TYR:OH	1:B:156:LYS:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:ARG:HB2	1:B:470:ARG:NH2	2.28	0.47
1:B:683:ARG:HG2	1:B:685:VAL:HG13	1.95	0.47
1:A:157:GLU:O	1:A:204:ARG:NH1	2.47	0.47
2:C:77:VAL:HB	2:C:96:LEU:HB3	1.95	0.47
2:C:74:ARG:C	2:C:76:GLN:H	2.16	0.47
1:A:391:LYS:O	1:A:393:LEU:N	2.47	0.47
1:B:448:VAL:HB	1:B:460:ILE:HB	1.95	0.47
1:A:560:LEU:C	1:A:562:GLN:H	2.18	0.47
2:D:513:SER:OG	2:D:533:CYS:SG	2.73	0.47
1:B:200:THR:HG22	1:B:229:LEU:O	2.15	0.47
1:B:370:LYS:O	1:B:374:GLN:CB	2.62	0.47
1:B:466:ASN:C	1:B:468:GLY:H	2.16	0.47
1:B:155:ARG:HB2	1:B:158:HIS:CG	2.50	0.47
1:B:487:LEU:HD23	1:B:487:LEU:HA	1.71	0.47
1:A:574:SER:HB2	1:A:659:TYR:CE2	2.50	0.47
2:D:316:PHE:O	2:D:327:ALA:N	2.37	0.47
1:A:683:ARG:O	1:A:684:HIS:ND1	2.46	0.47
2:C:101:ARG:O	2:C:105:ARG:HG3	2.14	0.47
1:B:126:ARG:NH1	1:B:210:GLU:HG3	2.30	0.47
2:C:226:ALA:O	2:C:227:ILE:HG13	2.15	0.47
1:B:348:ARG:O	1:B:351:PRO:HD3	2.15	0.47
1:A:42:ARG:HG3	1:A:509:ARG:NH2	2.30	0.47
1:A:126:ARG:NH2	1:A:207:MET:O	2.41	0.47
2:D:363:PRO:O	2:D:364:LYS:HD3	2.15	0.47
1:B:405:ASP:OD1	1:B:405:ASP:N	2.48	0.46
1:A:383:LEU:HD23	1:A:383:LEU:H	1.78	0.46
2:C:358:PRO:HD2	2:C:361:LYS:HD2	1.97	0.46
1:A:495:ASN:OD1	1:A:495:ASN:N	2.44	0.46
1:B:349:VAL:HG13	1:B:350:LYS:HG2	1.97	0.46
2:C:313:ILE:HG22	2:C:424:ILE:HD11	1.97	0.46
1:B:141:LEU:HB3	1:B:146:LEU:HA	1.97	0.46
2:D:147:TYR:CE2	2:D:202:MET:HE1	2.49	0.46
2:D:167:PRO:HG3	2:D:174:ASN:HB3	1.97	0.46
1:A:612:ASP:OD1	1:A:612:ASP:N	2.47	0.46
2:C:227:ILE:HD11	2:C:302:ASP:HA	1.96	0.46
1:B:226:SER:O	1:B:228:GLN:N	2.40	0.46
1:B:157:GLU:O	1:B:204:ARG:NH1	2.48	0.46
1:A:569:GLN:HA	1:A:570:PRO:HA	1.62	0.46
1:B:568:VAL:HG22	1:B:584:LEU:HG	1.98	0.46
2:C:341:LYS:HA	2:C:366:ARG:HH21	1.80	0.46
1:A:183:ALA:O	1:A:206:LEU:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:LYS:HB2	1:B:394:GLY:HA2	1.98	0.45
1:A:463:ASP:O	1:A:471:PRO:HA	2.16	0.45
2:C:74:ARG:HB2	2:C:121:PHE:CE1	2.51	0.45
1:B:490:LEU:HD22	1:B:499:LEU:HD11	1.98	0.45
1:A:579:GLN:HA	1:A:619:SER:O	2.16	0.45
2:C:432:PRO:HG3	2:C:555:GLN:OE1	2.16	0.45
1:B:239:PHE:CD1	1:B:242:PHE:HB2	2.50	0.45
2:D:190:ASP:OD1	2:D:193:ALA:N	2.50	0.45
2:D:406:ILE:C	2:D:408:ASP:H	2.20	0.45
2:D:431:GLY:HA2	2:D:531:PRO:HB2	1.98	0.45
1:A:54:LEU:HD23	1:A:55:VAL:N	2.31	0.45
1:A:700:VAL:HG13	1:A:705:ASP:CB	2.46	0.45
2:C:188:VAL:HG11	2:C:193:ALA:HA	1.98	0.45
1:B:555:ARG:HD2	1:B:590:PRO:HG3	1.98	0.45
2:C:500:TYR:CZ	2:C:509:ARG:HG3	2.52	0.45
2:C:426:VAL:HG22	2:C:439:ILE:HG12	1.99	0.45
1:B:203:SER:HB3	1:B:227:SER:HB2	1.99	0.45
2:C:243:GLU:OE1	2:C:243:GLU:N	2.45	0.45
1:A:298:PHE:HZ	1:A:372:ARG:CB	2.30	0.44
1:A:298:PHE:HZ	1:A:372:ARG:HB3	1.82	0.44
1:B:58:GLU:O	1:B:494:PRO:HB3	2.17	0.44
2:D:42:PRO:HG2	2:D:509:ARG:HB3	1.98	0.44
1:A:574:SER:OG	1:A:576:THR:HG23	2.17	0.44
2:C:165:ARG:NH2	2:C:201:SER:HB3	2.21	0.44
1:A:348:ARG:HE	1:A:348:ARG:HB3	1.63	0.44
1:A:113:ASN:OD1	1:A:132:SER:N	2.45	0.44
1:A:268:THR:CG2	1:A:277:PHE:H	2.30	0.44
1:A:625:VAL:HA	1:A:628:ILE:HD12	1.98	0.44
1:B:254:GLN:O	1:B:287:VAL:HG22	2.18	0.44
1:A:207:MET:SD	1:A:215:MET:HA	2.57	0.44
1:A:324:LEU:HA	1:A:327:GLN:HB2	1.99	0.44
2:D:155:TYR:OH	2:D:158:GLU:HA	2.16	0.44
1:A:481:GLN:OE1	1:A:505:LYS:HB2	2.17	0.44
1:A:632:GLN:O	1:A:632:GLN:HG3	2.18	0.44
1:B:675:PHE:HB3	1:B:676:PRO:HD2	2.00	0.44
1:A:261:LEU:HD11	1:A:278:PHE:HB3	2.00	0.44
1:A:402:ILE:HG22	1:A:403:ASP:O	2.18	0.44
1:A:537:LEU:HD13	1:A:555:ARG:NH1	2.33	0.44
1:B:54:LEU:HD23	1:B:55:VAL:N	2.33	0.43
1:B:191:ILE:HD12	1:B:193:GLY:N	2.33	0.43
2:C:223:PHE:HA	2:C:237:PHE:CB	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:699:ARG:NH1	1:A:701:ASN:ND2	2.66	0.43
2:D:65:ILE:HD12	2:D:70:TYR:HE2	1.83	0.43
1:A:286:CYS:HB2	1:A:289:ASP:HB2	1.99	0.43
1:B:116:LYS:HG2	1:B:166:ALA:HA	1.99	0.43
1:A:200:THR:HG22	1:A:229:LEU:O	2.18	0.43
1:A:369:ILE:O	1:A:373:ILE:HG23	2.18	0.43
2:C:281:ARG:HG2	2:C:282:LEU:N	2.33	0.43
2:C:283:ASN:OD1	2:C:285:SER:HB3	2.18	0.43
1:B:687:THR:HG21	1:B:692:ASP:HB2	2.00	0.43
1:B:426:LEU:O	1:B:472:ALA:HB3	2.19	0.43
2:D:220:GLU:HB2	2:D:240:ILE:HD12	2.01	0.43
2:D:349:THR:OG1	2:D:352:SER:HB3	2.19	0.43
2:D:489:SER:O	2:D:490:LEU:HD23	2.18	0.43
2:D:490:LEU:HD21	2:D:501:VAL:HG13	2.00	0.43
1:A:53:HIS:O	1:A:66:GLY:N	2.46	0.43
2:D:221:PRO:HB3	2:D:239:GLU:HB3	2.01	0.43
2:C:268:ARG:HE	2:C:387:ASP:CG	2.21	0.43
2:C:300:ILE:HD11	2:C:312:VAL:HB	2.00	0.43
2:C:62:MET:HB2	2:C:69:LEU:HD11	2.01	0.43
1:B:415:LEU:HD12	1:B:415:LEU:HA	1.85	0.43
1:A:234:ASP:O	1:A:237:SER:OG	2.27	0.43
2:D:108:CYS:HB2	2:D:140:ALA:HB1	2.00	0.43
2:C:96:LEU:HD11	2:C:148:TYR:CG	2.54	0.43
1:B:569:GLN:HA	1:B:570:PRO:HA	1.77	0.43
1:A:383:LEU:HD12	1:A:389:LEU:HD11	2.01	0.43
2:D:25:GLU:HG2	2:D:26:ASP:N	2.34	0.43
1:B:393:LEU:HD21	2:D:192:LEU:HD22	2.01	0.42
2:D:436:TYR:HB3	2:D:452:LEU:HD11	1.99	0.42
1:A:311:LEU:HB2	1:A:342:ALA:HB3	2.00	0.42
2:D:228:GLU:HG3	2:D:260:LYS:HE2	2.00	0.42
2:C:245:ASN:C	2:C:247:LEU:H	2.23	0.42
2:D:235:PHE:HB2	2:D:256:ALA:HB3	2.01	0.42
1:A:470:ARG:CZ	1:A:470:ARG:HB2	2.50	0.42
2:D:163:LEU:HD12	2:D:163:LEU:HA	1.72	0.42
1:B:96:TYR:O	2:D:268:ARG:HG2	2.20	0.42
1:B:174:ILE:HG12	1:B:251:ARG:HD2	2.01	0.42
1:A:126:ARG:HH11	1:A:210:GLU:HG3	1.85	0.42
1:A:620:PRO:HB2	1:A:625:VAL:HG23	2.00	0.42
2:C:362:VAL:HG11	2:C:366:ARG:HH11	1.84	0.42
1:B:92:ASN:OD1	1:B:93:GLU:N	2.53	0.42
1:B:324:LEU:HD23	1:B:324:LEU:HA	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:LEU:HB3	1:B:415:LEU:HD12	2.00	0.42
1:B:492:LEU:HD12	1:B:499:LEU:HD13	2.02	0.42
2:D:297:LEU:HD13	2:D:316:PHE:CZ	2.55	0.42
2:D:353:VAL:HG22	2:C:353:VAL:HG22	2.00	0.42
1:B:42:ARG:HG3	1:B:509:ARG:NE	2.35	0.42
1:A:555:ARG:HE	1:A:555:ARG:HB3	1.50	0.42
1:A:569:GLN:HB2	1:A:583:VAL:HG13	2.01	0.42
1:A:674:SER:HB3	4:A:1002:NAG:C8	2.50	0.42
2:D:65:ILE:HG22	2:D:66:ARG:HG2	2.01	0.42
2:D:230:GLY:O	2:D:260:LYS:HE3	2.19	0.42
2:C:209:ARG:NE	2:C:210:THR:O	2.48	0.42
2:D:497:HIS:CE1	2:D:513:SER:H	2.37	0.41
1:B:78:LEU:HD21	1:B:500:TYR:HD1	1.85	0.41
2:D:288:GLY:HA3	2:C:321:ASN:HD22	1.85	0.41
2:C:107:ASN:O	2:C:111:LYS:HG3	2.20	0.41
2:C:460:LEU:HA	2:C:460:LEU:HD23	1.85	0.41
1:A:191:ILE:HD12	1:A:193:GLY:N	2.35	0.41
1:A:466:ASN:HA	1:A:467:PRO:HD3	1.94	0.41
2:D:275:THR:O	2:D:393:ILE:HD13	2.20	0.41
2:D:490:LEU:HD22	2:D:501:VAL:HA	2.02	0.41
1:B:223:GLU:HB3	1:B:224:PHE:CE2	2.56	0.41
1:A:492:LEU:HD23	1:A:496:HIS:HA	2.03	0.41
1:A:678:HIS:ND1	1:A:701:ASN:OD1	2.53	0.41
2:D:347:GLN:HB2	2:D:354:TRP:CD2	2.55	0.41
2:C:497:HIS:CD2	2:C:512:LEU:HB2	2.56	0.41
1:B:161:SER:OG	1:B:163:VAL:HG22	2.21	0.41
1:B:490:LEU:HD23	1:B:490:LEU:HA	1.90	0.41
1:A:382:LYS:HB2	1:A:393:LEU:O	2.20	0.41
1:A:426:LEU:O	1:A:472:ALA:HB3	2.21	0.41
2:D:41:TYR:CD2	2:D:510:ILE:HD13	2.55	0.41
2:C:241:ALA:HB2	2:C:252:TYR:CB	2.50	0.41
1:B:650:LYS:HE3	1:B:650:LYS:HB2	1.90	0.41
1:A:372:ARG:NH2	1:A:382:LYS:O	2.54	0.41
1:A:622:ALA:HA	1:A:625:VAL:HB	2.02	0.41
2:D:315:VAL:HG23	2:D:424:ILE:HD12	2.03	0.41
2:C:26:ASP:OD2	2:C:416:ARG:HB2	2.21	0.41
2:C:37:TYR:HD1	2:C:514:ARG:NH2	2.19	0.41
2:D:533:CYS:O	2:D:555:GLN:NE2	2.53	0.41
2:C:307:ASN:OD1	2:C:456:SER:HB2	2.20	0.41
1:B:311:LEU:HB2	1:B:342:ALA:HB3	2.01	0.41
1:A:82:ARG:HH21	1:A:82:ARG:HD2	1.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:GLN:HG2	1:A:182:GLN:H	1.86	0.41
1:A:426:LEU:HB3	1:A:472:ALA:HB2	2.02	0.41
2:C:535:TRP:CZ2	2:C:539:GLY:HA2	2.56	0.41
1:B:283:VAL:HA	1:B:296:VAL:O	2.21	0.41
1:A:383:LEU:HD21	1:A:393:LEU:HG	2.03	0.41
1:A:644:SER:HB2	1:A:651:PHE:CE2	2.56	0.41
2:D:183:LEU:O	2:D:200:ARG:HA	2.21	0.41
1:B:73:LYS:O	1:B:81:LEU:HB2	2.21	0.40
1:A:448:VAL:HB	1:A:460:ILE:HB	2.02	0.40
1:A:579:GLN:HE21	1:A:621:SER:HB3	1.86	0.40
1:A:621:SER:O	1:A:624:GLU:N	2.53	0.40
2:D:289:ASP:O	2:C:249:LYS:HB3	2.22	0.40
2:C:299:SER:OG	2:C:424:ILE:HG22	2.21	0.40
1:B:42:ARG:HH12	4:B:1001:NAG:H81	1.87	0.40
1:A:378:ARG:HD3	1:A:380:GLU:OE2	2.22	0.40
2:D:55:HIS:O	2:D:55:HIS:CG	2.74	0.40
2:C:291:PHE:CE2	3:G:1:NAG:H5	2.56	0.40
2:C:514:ARG:NE	2:C:517:ARG:HB2	2.36	0.40
1:B:92:ASN:HB2	1:B:108:LEU:HA	2.04	0.40
1:B:647:THR:HG23	1:B:649:LYS:H	1.86	0.40
1:B:699:ARG:HG2	1:B:701:ASN:HD21	1.86	0.40
1:B:78:LEU:HD21	1:B:500:TYR:CD1	2.57	0.40
1:B:152:PRO:HB2	1:B:158:HIS:ND1	2.37	0.40
1:B:183:ALA:HB3	1:B:206:LEU:HB2	2.03	0.40
2:C:218:ILE:HG12	2:C:221:PRO:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	668/694 (96%)	596 (89%)	67 (10%)	5 (1%)	22	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	668/694 (96%)	593 (89%)	64 (10%)	11 (2%)	9	45
2	C	517/552 (94%)	456 (88%)	58 (11%)	3 (1%)	25	65
2	D	519/552 (94%)	454 (88%)	59 (11%)	6 (1%)	13	50
All	All	2372/2492 (95%)	2099 (88%)	248 (10%)	25 (1%)	14	52

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	47	SER
1	B	106	HIS
1	B	181	GLY
1	B	273	ALA
1	A	684	HIS
2	D	466	LEU
2	D	485	ARG
2	D	543	ARG
2	C	525	CYS
1	B	108	LEU
1	A	348	ARG
1	A	630	ARG
1	B	630	ARG
2	D	512	LEU
1	B	240	PRO
1	A	240	PRO
2	D	206	SER
2	C	519	GLY
1	B	148	LYS
1	B	347	ASN
1	A	561	LEU
1	B	105	PRO
2	C	408	ASP
1	B	467	PRO
2	D	374	GLY

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	580/596 (97%)	555 (96%)	25 (4%)	29	54
1	B	580/596 (97%)	557 (96%)	23 (4%)	31	56
2	C	461/482 (96%)	444 (96%)	17 (4%)	34	59
2	D	463/482 (96%)	455 (98%)	8 (2%)	60	78
All	All	2084/2156 (97%)	2011 (96%)	73 (4%)	36	60

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	70	ARG
1	B	82	ARG
1	B	116	LYS
1	B	196	GLU
1	B	204	ARG
1	B	207	MET
1	B	220	TYR
1	B	235	THR
1	B	239	PHE
1	B	271	ASP
1	B	302	CYS
1	B	383	LEU
1	B	391	LYS
1	B	429	ASP
1	B	440	TYR
1	B	446	THR
1	B	463	ASP
1	B	528	ARG
1	B	543	ARG
1	B	544	ARG
1	B	614	ARG
1	B	649	LYS
1	B	695	PHE
1	A	70	ARG
1	A	204	ARG
1	A	207	MET
1	A	233	SER
1	A	239	PHE
1	A	271	ASP
1	A	276	HIS
1	A	302	CYS

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Mol	Chain	Res	Type
1	A	343	GLN
1	A	378	ARG
1	A	429	ASP
1	A	440	TYR
1	A	446	THR
1	A	543	ARG
1	A	544	ARG
1	A	562	GLN
1	A	582	LEU
1	A	610	LEU
1	A	612	ASP
1	A	614	ARG
1	A	619	SER
1	A	636	ARG
1	A	649	LYS
1	A	655	ASP
1	A	695	PHE
2	D	27	ASP
2	D	37	TYR
2	D	87	GLN
2	D	163	LEU
2	D	232	TYR
2	D	247	LEU
2	D	456	SER
2	D	517	ARG
2	C	56	ARG
2	C	87	GLN
2	C	95	LYS
2	C	104	ASP
2	C	201	SER
2	C	202	MET
2	C	257	ARG
2	C	312	VAL
2	C	413	THR
2	C	418	ARG
2	C	428	ARG
2	C	460	LEU
2	C	462	ASP
2	C	529	ARG
2	C	540	VAL
2	C	554	GLU
2	C	567	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	497	HIS
2	C	321	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 ⓘ

10 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	NAG	E	1	3,2	14,14,15	0.68	1 (7%)	17,19,21	0.49	0
3	NAG	E	2	3	14,14,15	0.47	0	17,19,21	0.44	0
3	NAG	F	1	3,1	14,14,15	0.68	0	17,19,21	0.63	1 (5%)
3	NAG	F	2	3	14,14,15	0.57	0	17,19,21	0.48	0
3	NAG	G	1	3,2	14,14,15	0.62	0	17,19,21	0.59	1 (5%)
3	NAG	G	2	3	14,14,15	0.72	0	17,19,21	0.47	0
3	NAG	H	1	3,2	14,14,15	0.57	0	17,19,21	0.54	0
3	NAG	H	2	3	14,14,15	0.48	0	17,19,21	0.44	0
3	NAG	I	1	3,2	14,14,15	0.48	0	17,19,21	0.54	0
3	NAG	I	2	3	14,14,15	0.69	1 (7%)	17,19,21	0.46	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
3	NAG	E	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	1/6/23/26	0/1/1/1
3	NAG	G	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	NAG	O5-C1	-2.43	1.39	1.43
3	I	2	NAG	C1-C2	2.08	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	1	NAG	C1-O5-C5	2.06	114.99	112.19
3	G	1	NAG	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	2	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	F	1	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	1	0
3	I	1	NAG	2	0
3	E	1	NAG	1	0

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

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings
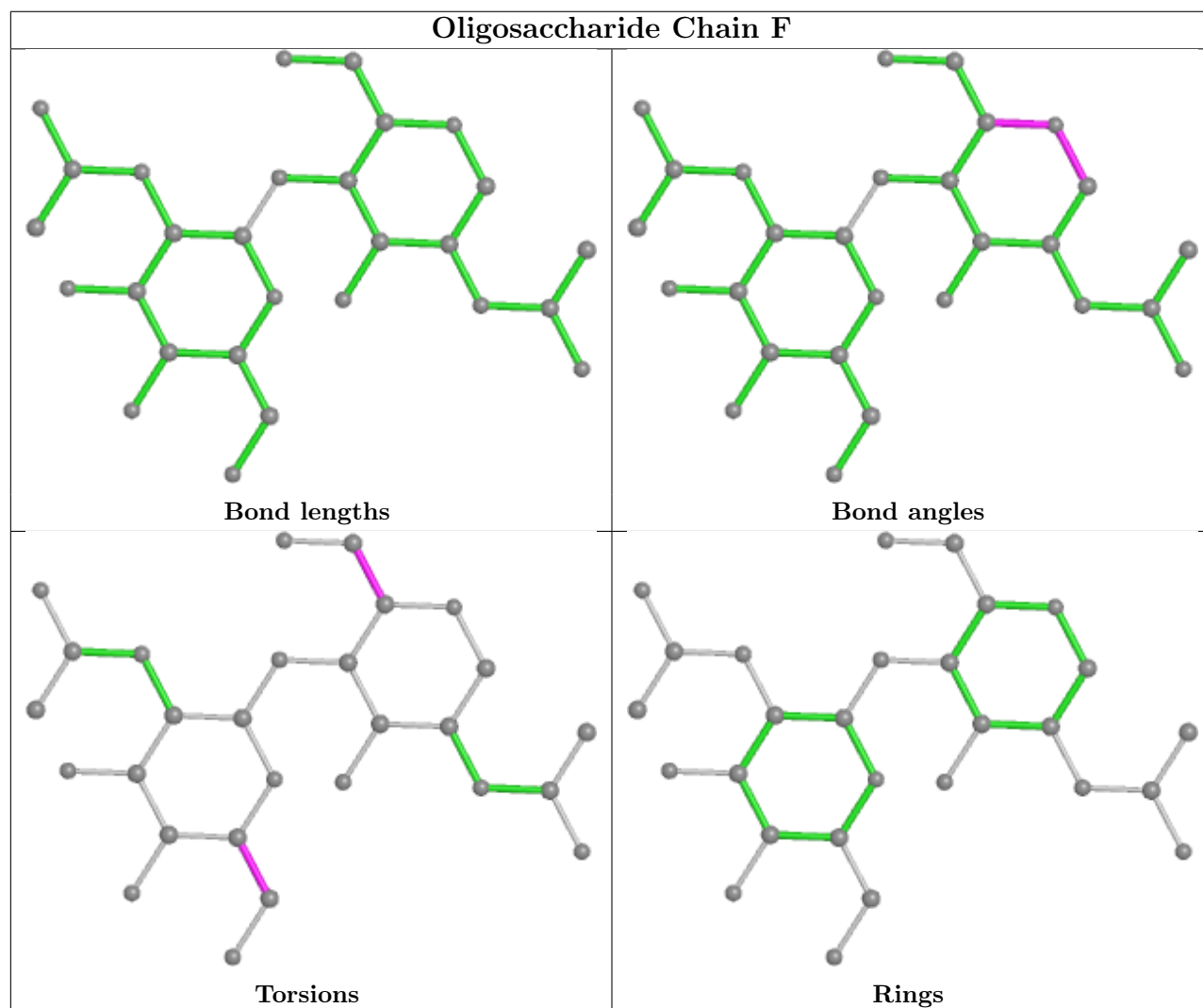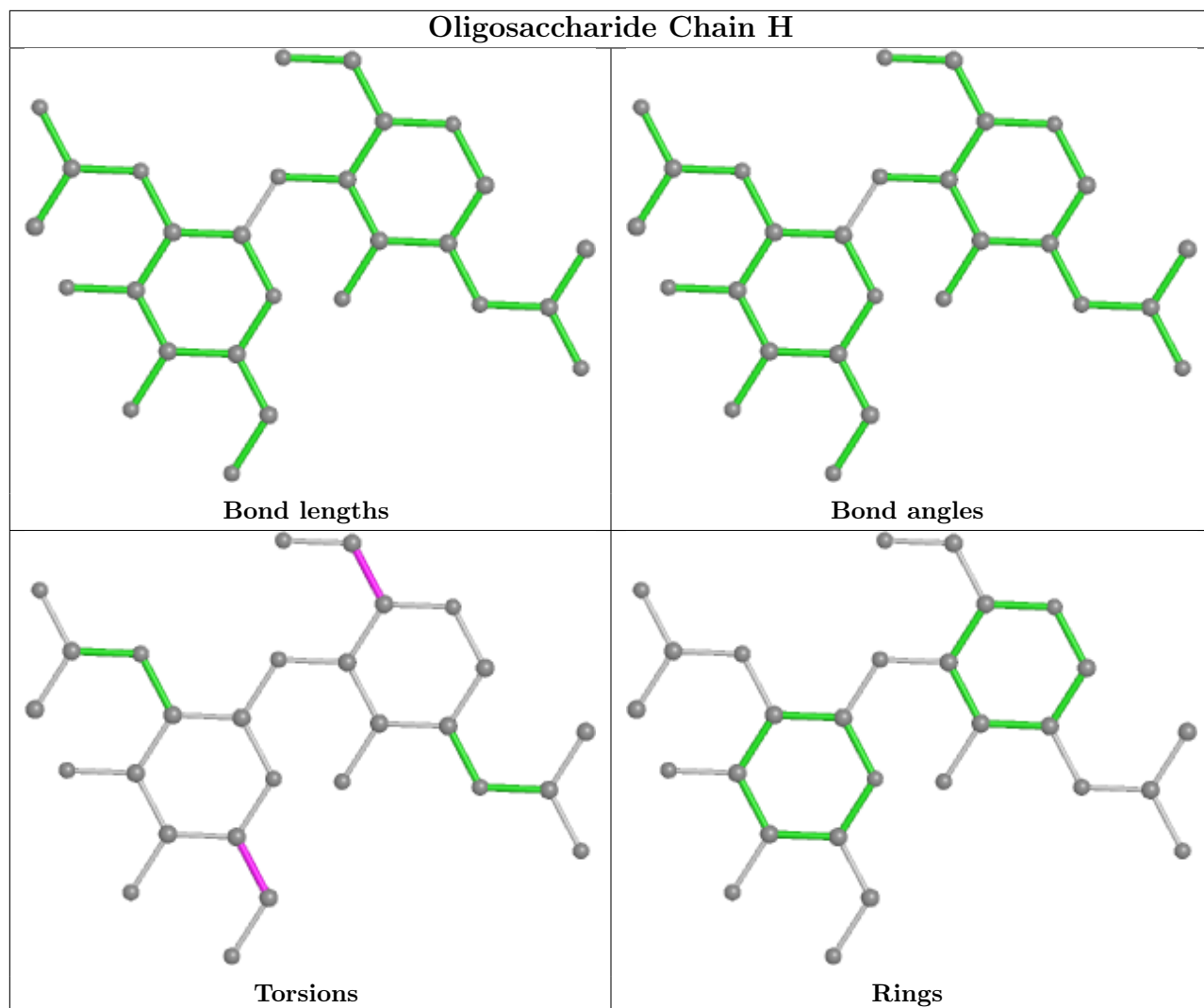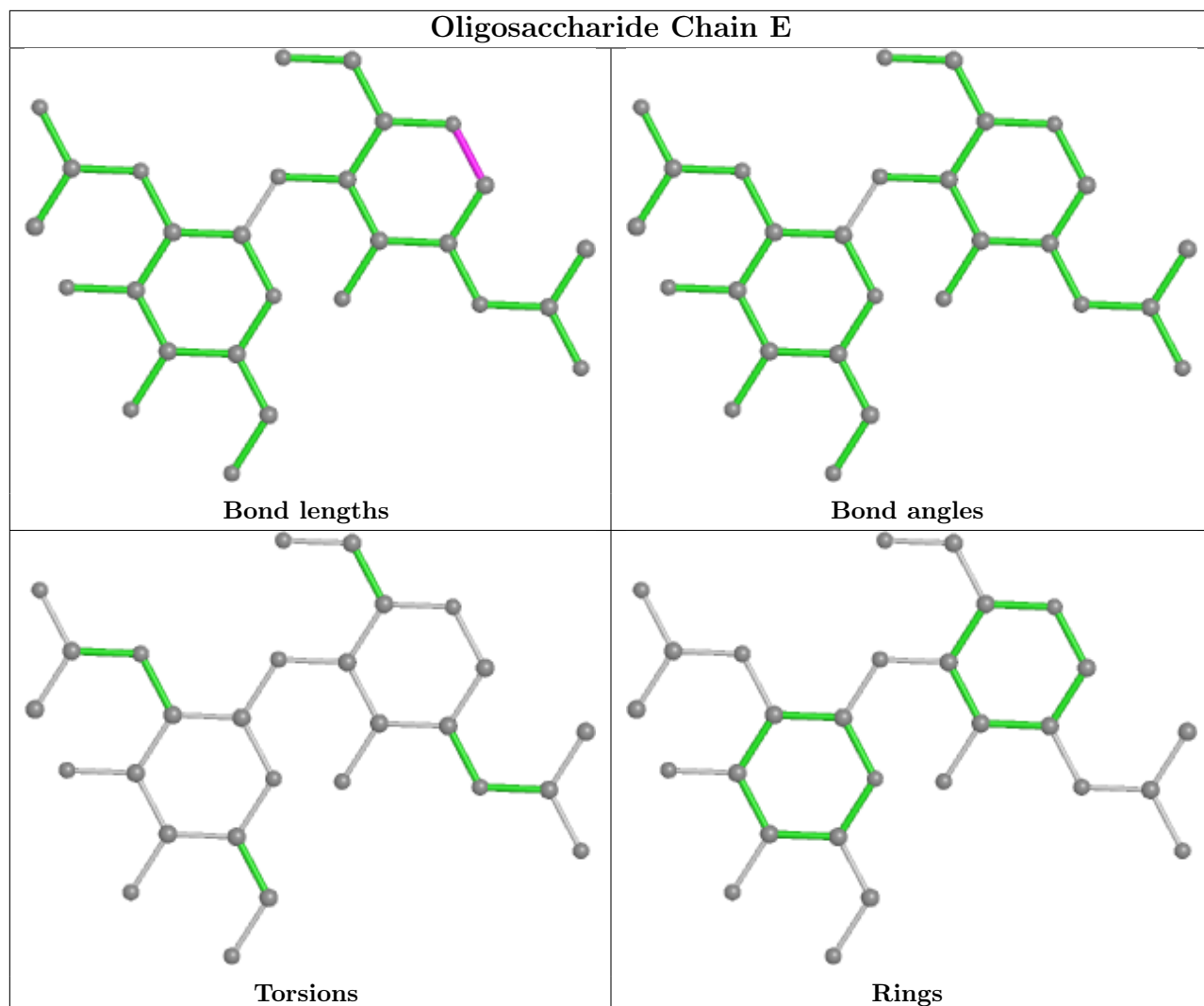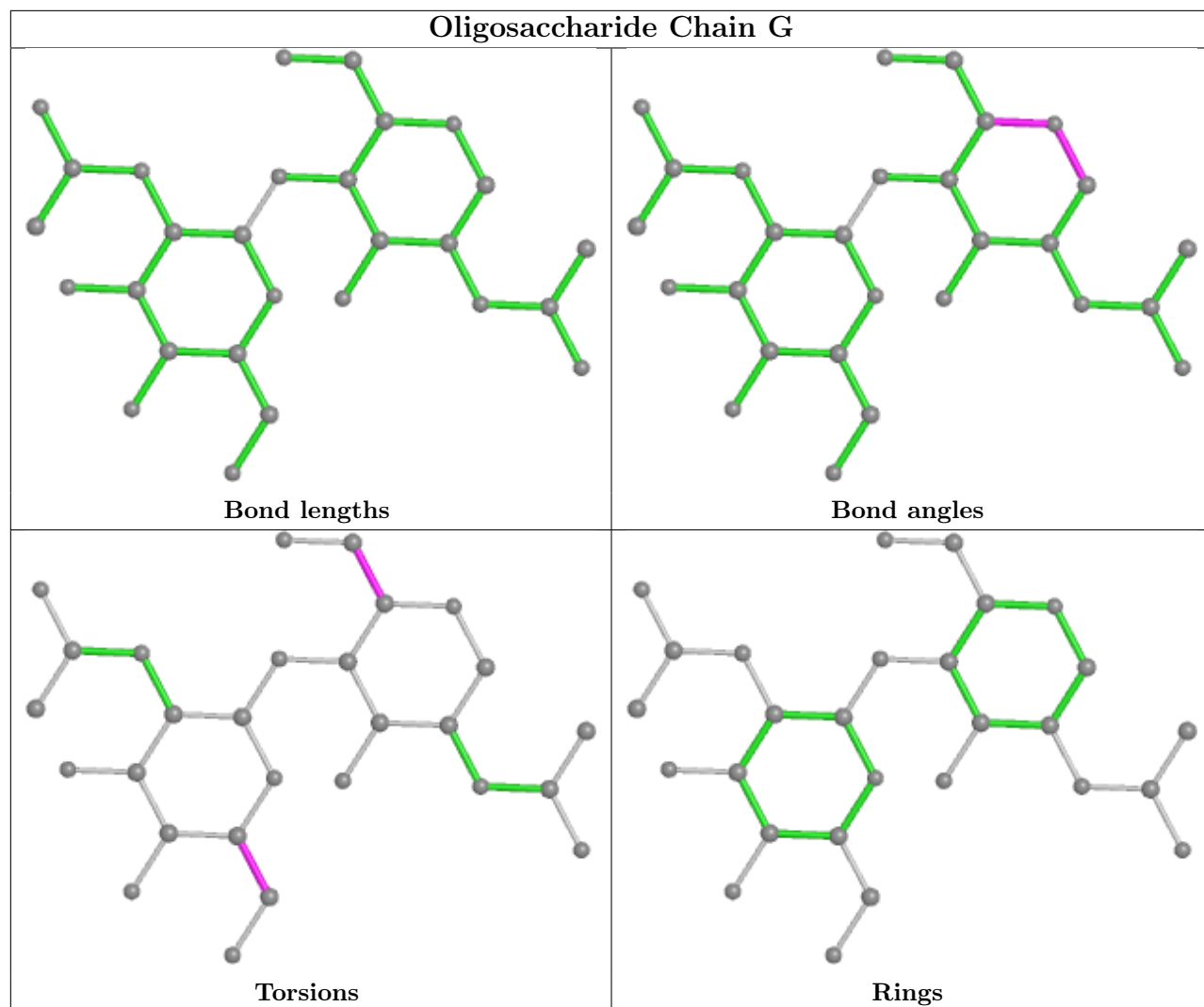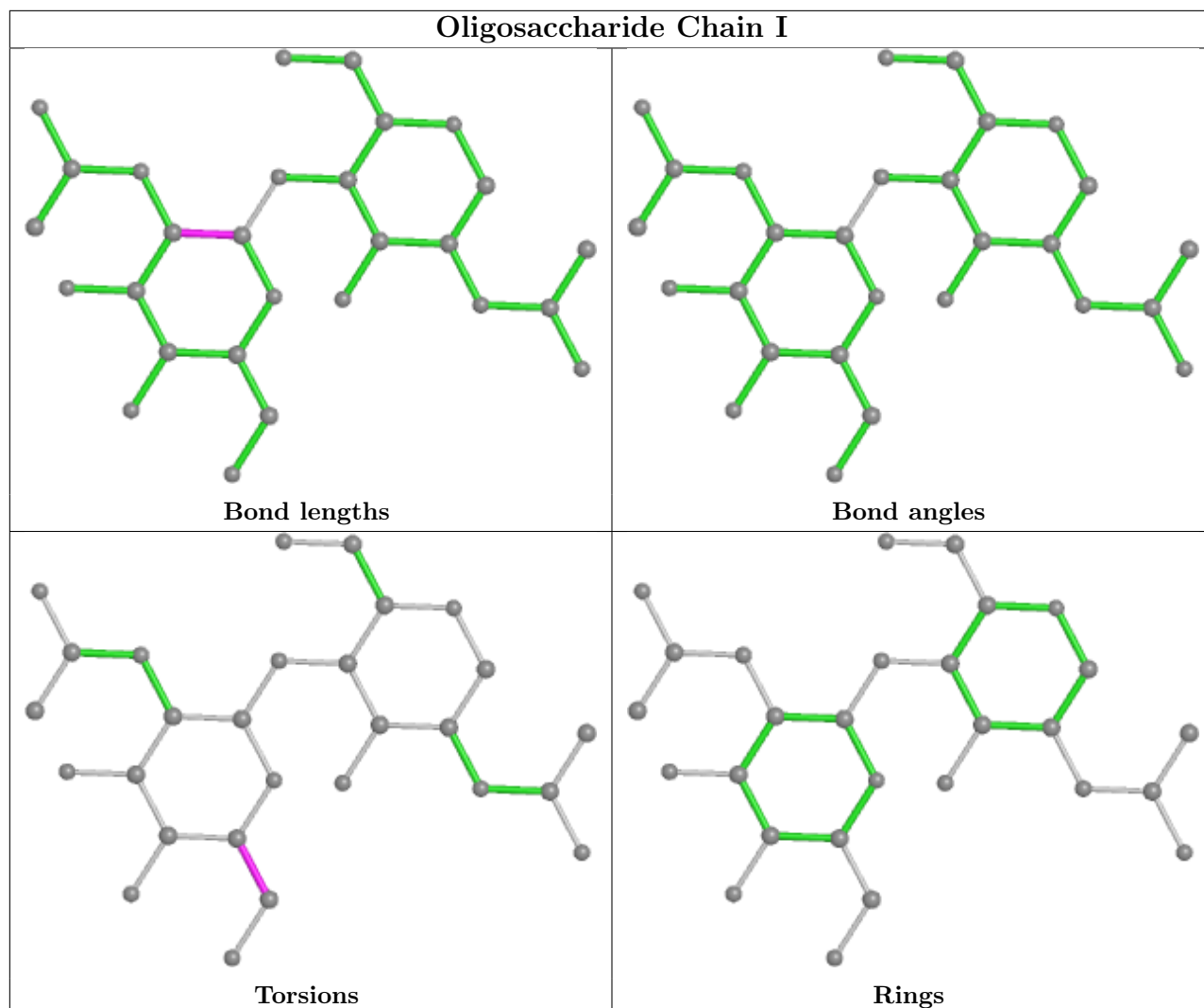
5.6 Ligand geometry (i)

4 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	NAG	A	1002	1	14,14,15	0.63	1 (7%)	17,19,21	0.67	0
4	NAG	B	1001	1	14,14,15	0.56	0	17,19,21	0.56	0
4	NAG	A	1001	1	14,14,15	0.37	0	17,19,21	0.48	0
4	NAG	B	1002	1	14,14,15	0.55	0	17,19,21	0.58	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	NAG	A	1002	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1001	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1001	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1002	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1002	NAG	O5-C1	2.08	1.47	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1001	NAG	O5-C5-C6-O6
4	B	1002	NAG	O5-C5-C6-O6
4	B	1002	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	NAG	2	0
4	B	1001	NAG	2	0

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

equivalents in the CSD to analyse the geometry.

Ligand NAG A 1002

Bond lengths

Bond angles

Torsions

Rings

Ligand NAG B 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand NAG A 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand NAG B 1002

Bond lengths

Bond angles

Torsions

Rings
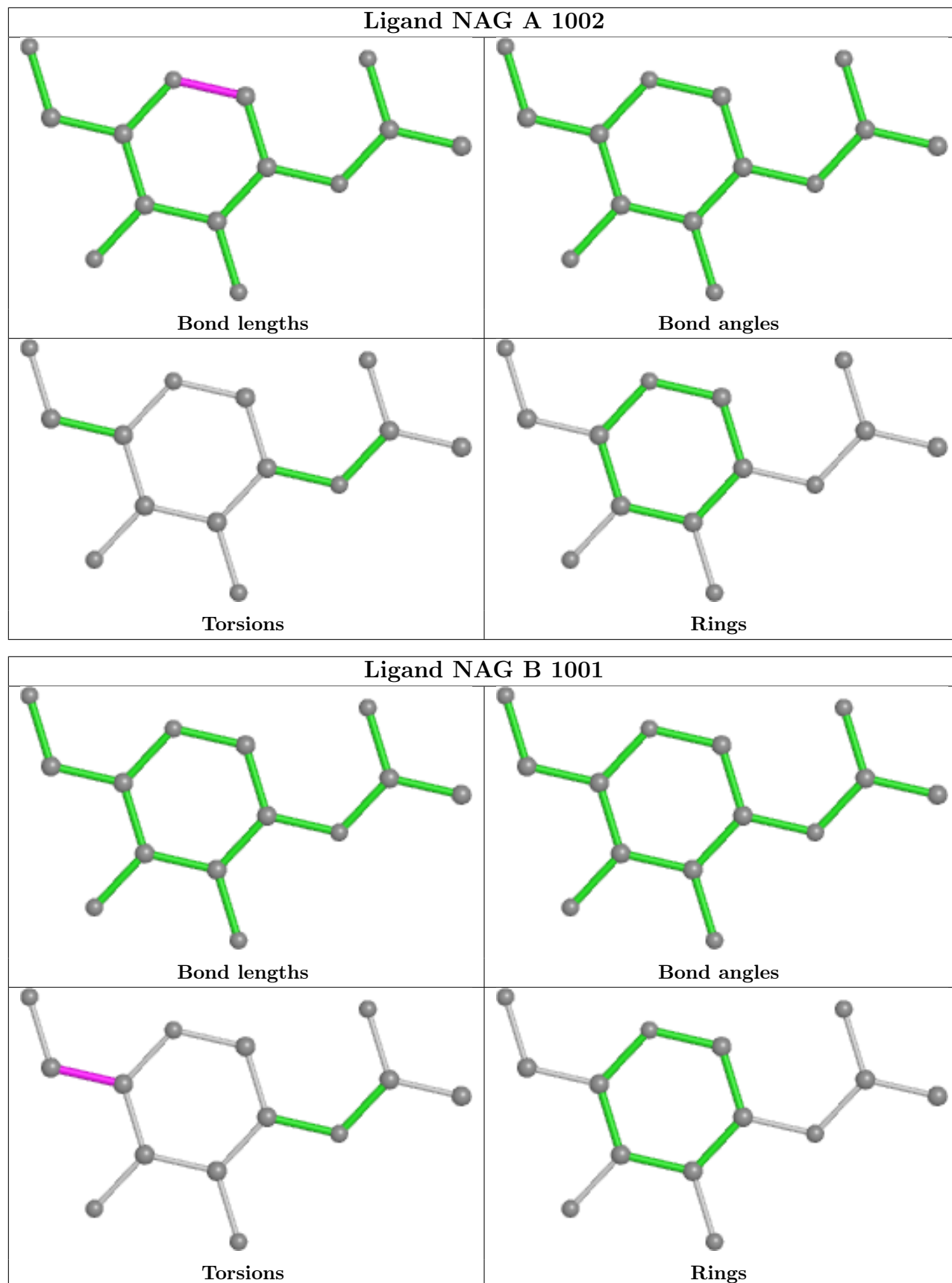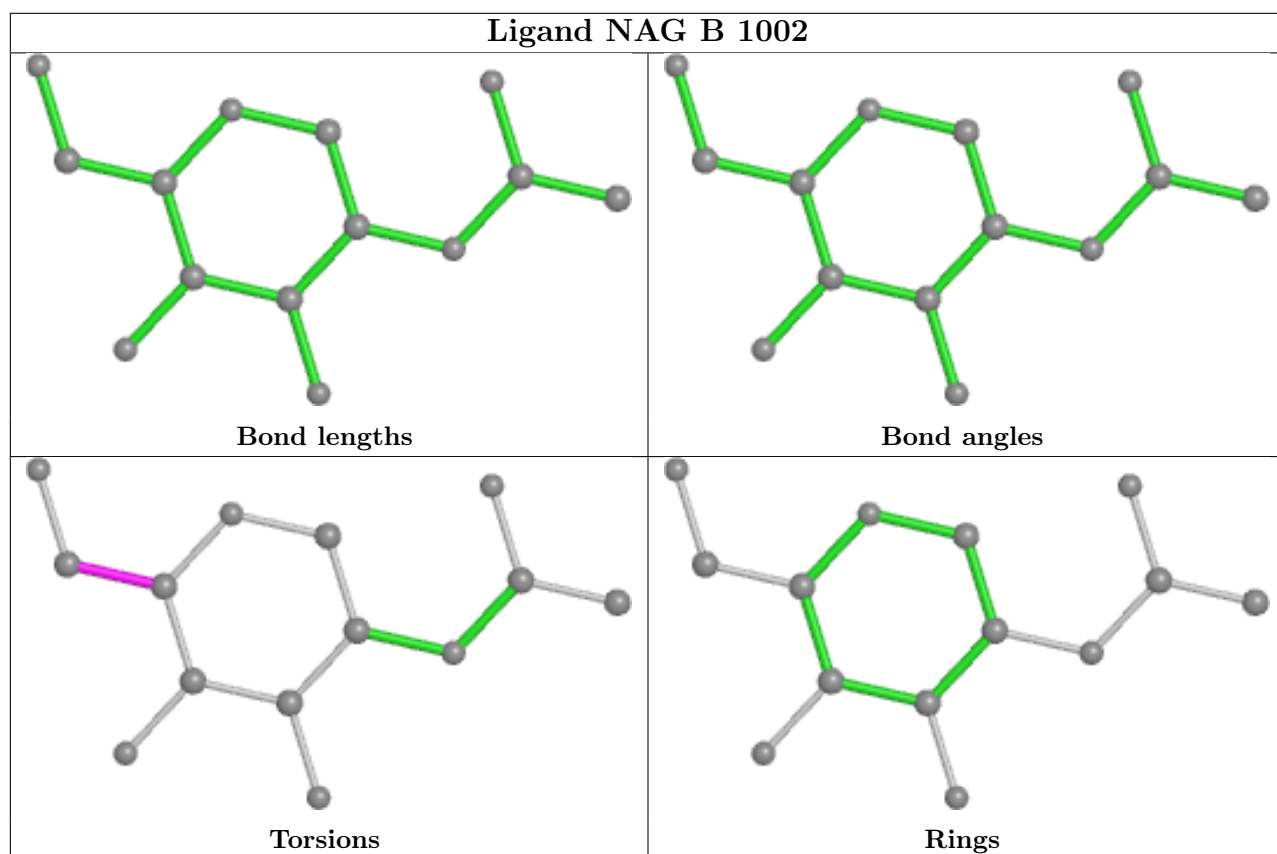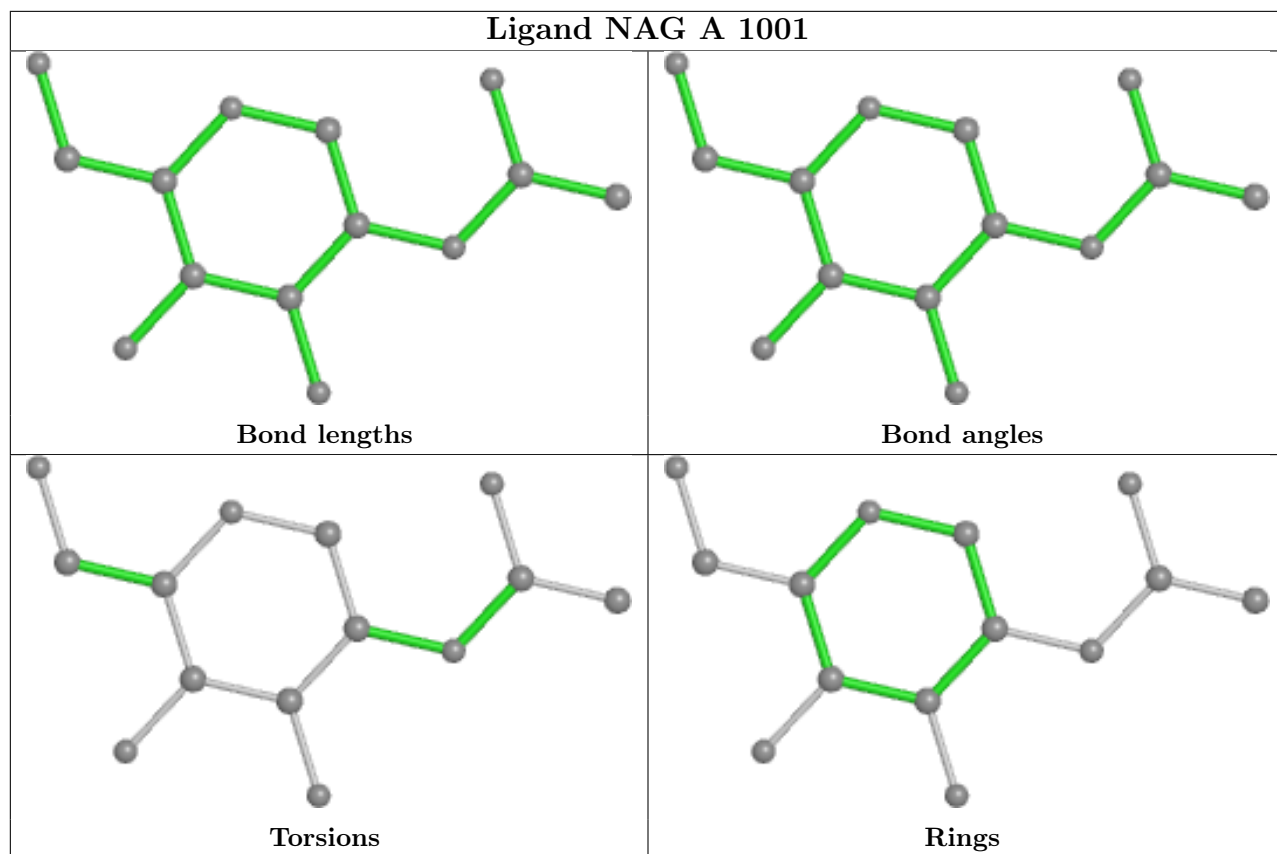
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	670/694 (96%)	-0.32	3 (0%)	92	87	146, 212, 261, 297	0
1	B	670/694 (96%)	-0.38	1 (0%)	95	94	146, 207, 281, 324	0
2	C	525/552 (95%)	-0.47	0	100	100	130, 176, 234, 280	0
2	D	527/552 (95%)	-0.42	0	100	100	133, 180, 240, 263	0
All	All	2392/2492 (95%)	-0.39	4 (0%)	95	93	130, 195, 265, 324	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	500	TYR	2.5
1	A	557	ALA	2.4
1	A	658	PHE	2.2
1	B	581	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

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	NAG	E	2	14/15	0.77	0.27	234,280,285,285	0
3	NAG	G	2	14/15	0.83	0.23	222,239,256,260	0
3	NAG	F	2	14/15	0.86	0.21	237,255,260,268	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	NAG	H	2	14/15	0.86	0.25	207,222,234,238	0
3	NAG	F	1	14/15	0.88	0.18	231,238,248,249	0
3	NAG	E	1	14/15	0.91	0.20	240,259,272,277	0
3	NAG	I	1	14/15	0.92	0.18	219,247,257,260	0
3	NAG	I	2	14/15	0.94	0.15	217,261,272,283	0
3	NAG	G	1	14/15	0.95	0.17	174,194,204,213	0
3	NAG	H	1	14/15	0.96	0.17	150,181,202,203	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 F:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
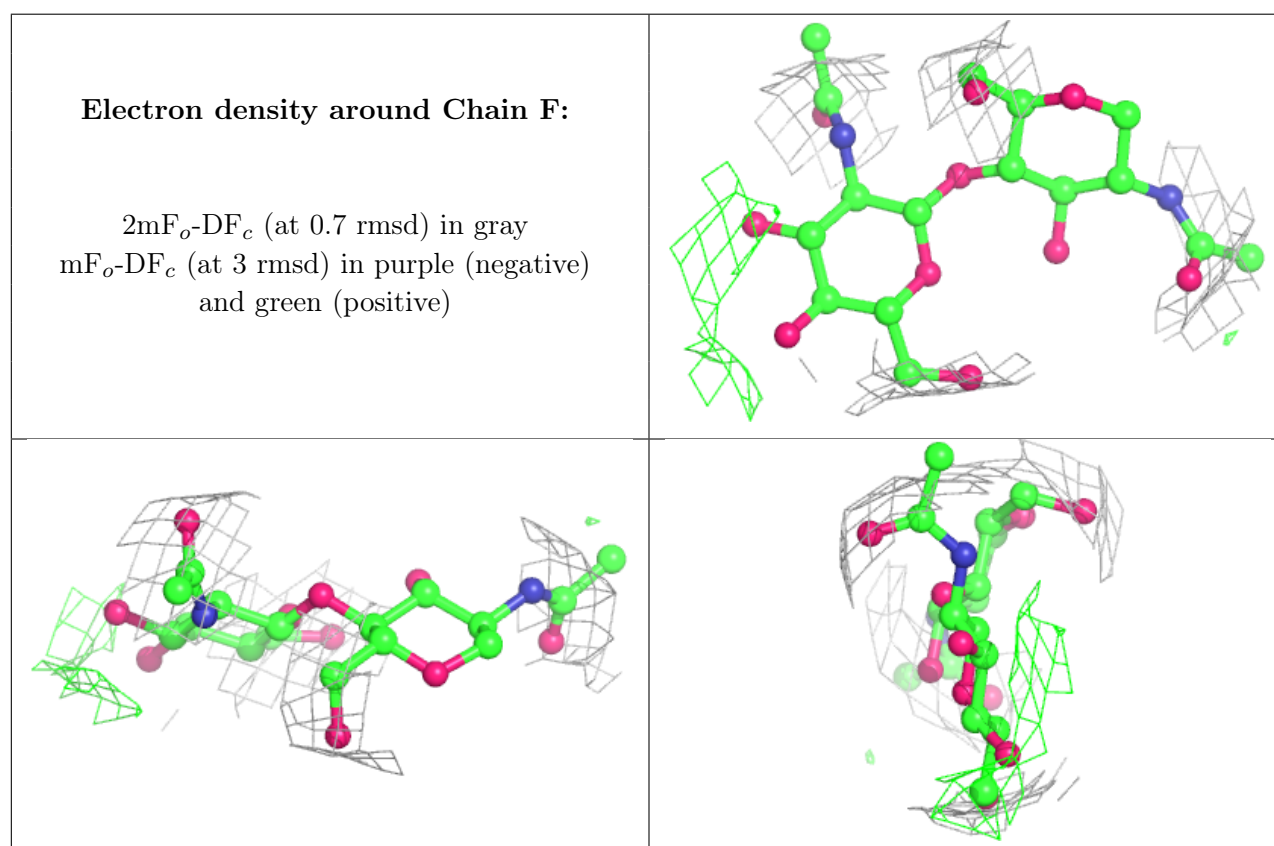
Electron density around Chain H:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
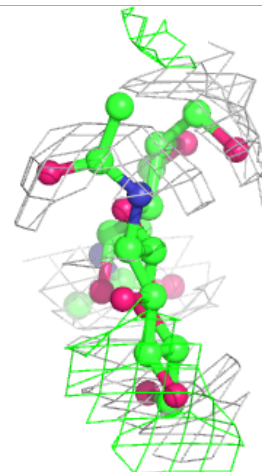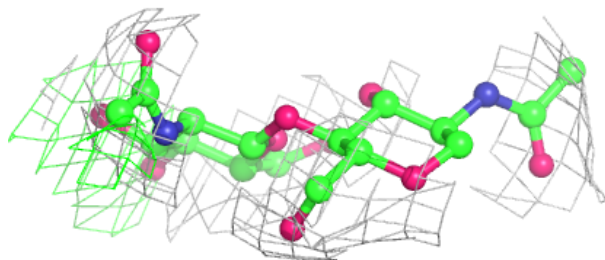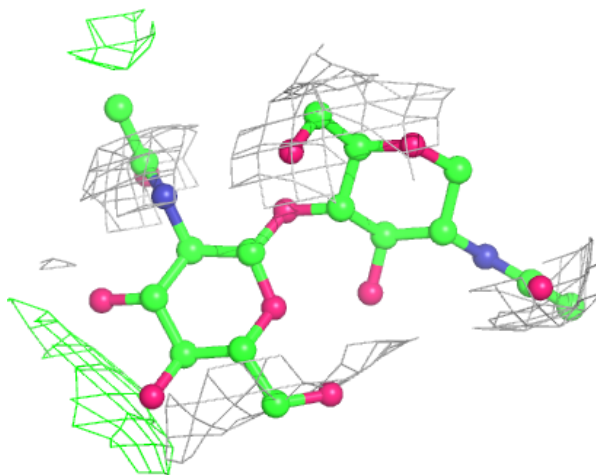
Electron density around Chain E:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
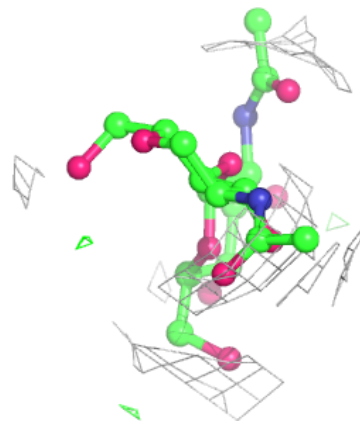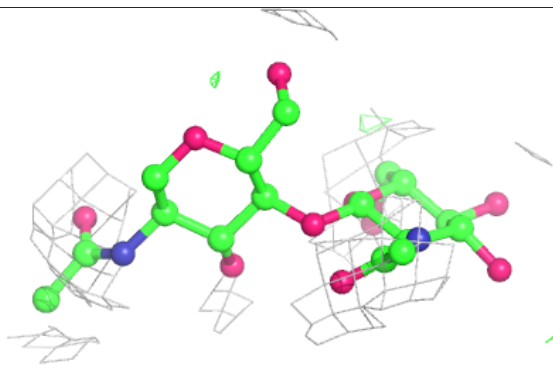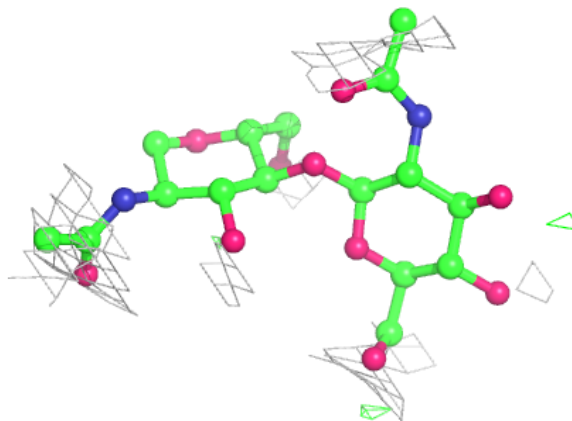
Electron density around Chain G:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
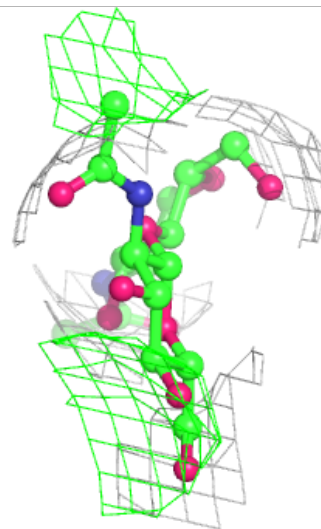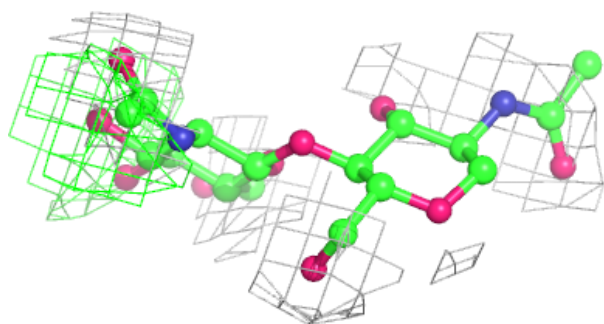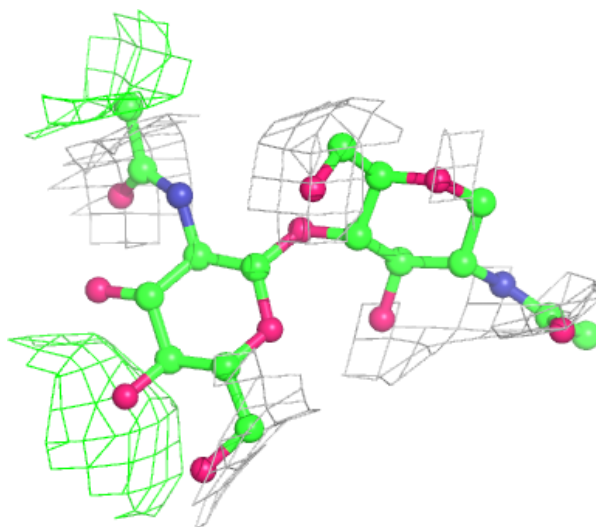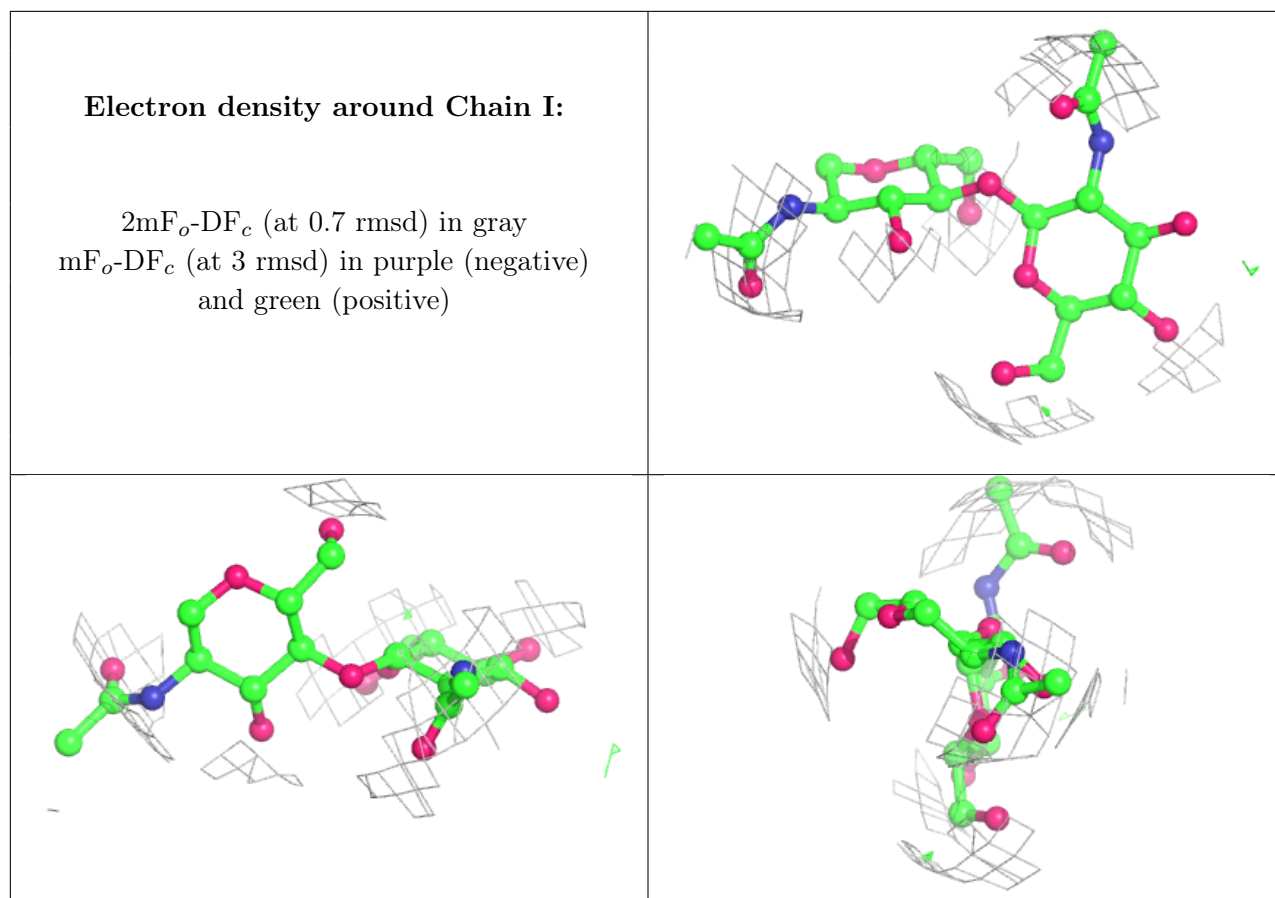
Electron density around Chain I:

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

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	NAG	B	1001	14/15	0.77	0.30	224,253,263,265	0
4	NAG	A	1001	14/15	0.81	0.26	254,269,272,273	0
4	NAG	A	1002	14/15	0.82	0.23	227,238,240,240	0
4	NAG	B	1002	14/15	0.87	0.15	225,236,242,245	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 NAG B 1001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
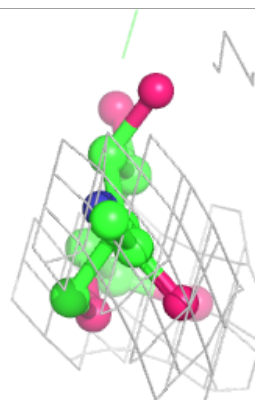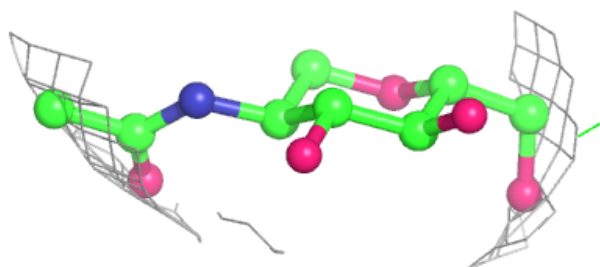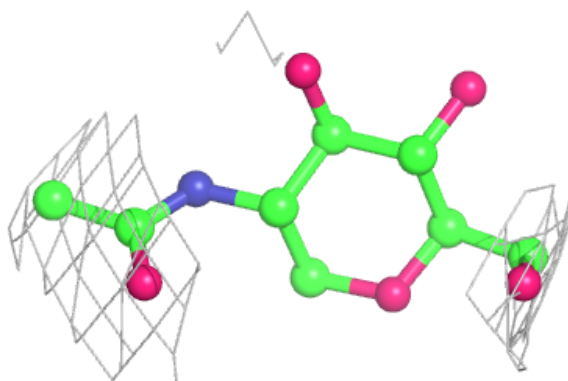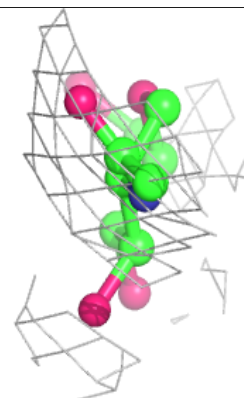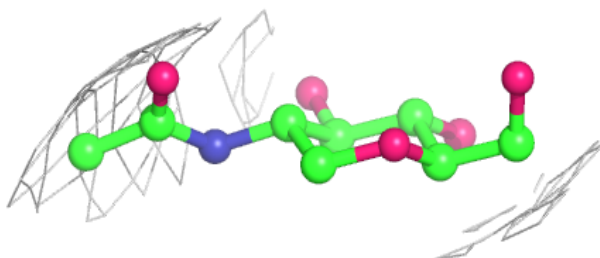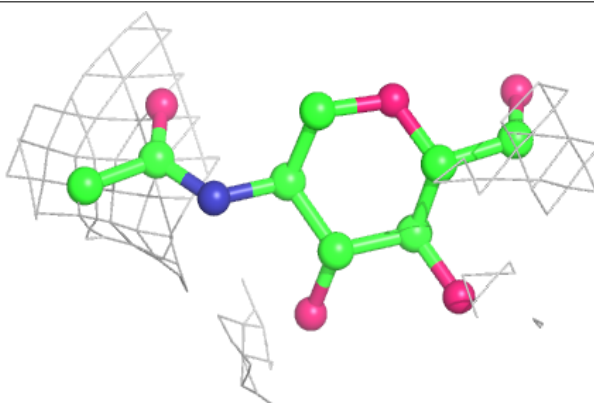and green (positive)
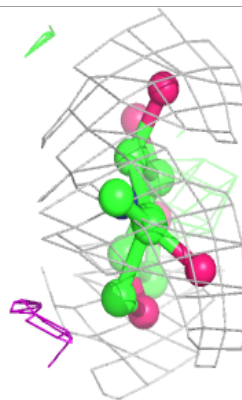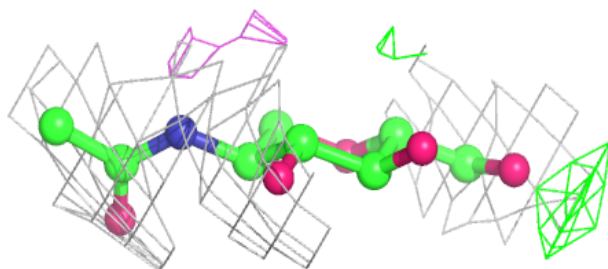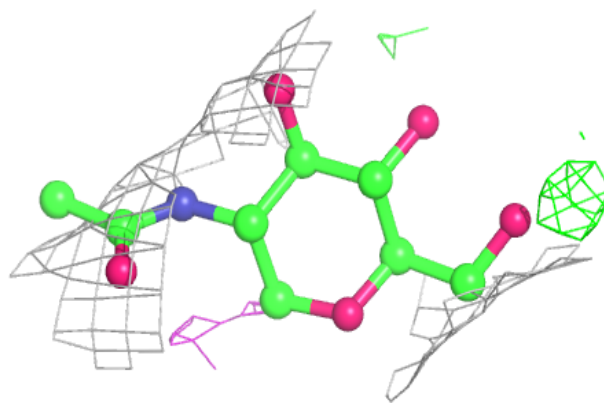
Electron density around NAG A 1001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
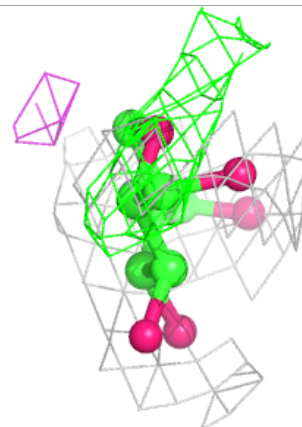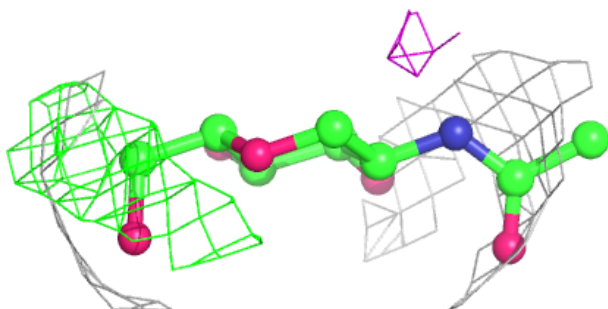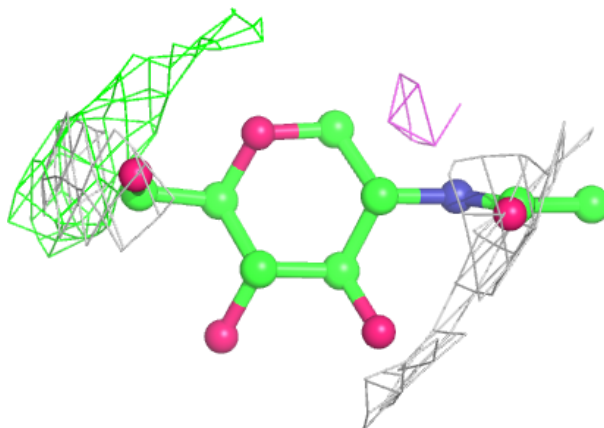
Electron density around NAG A 1002:

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

Electron density around NAG B 1002:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.