



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:32 AM UTC

PDB ID : 7NUP / pdb_00007nup
Title : Endoplasmic reticulum aminopeptidase 2 complexed with a mixed hydroxamic and sulfonyl ligand
Authors : Mpakali, A.; Giastas, P.; Stratikos, E.
Deposited on : 2021-03-12
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

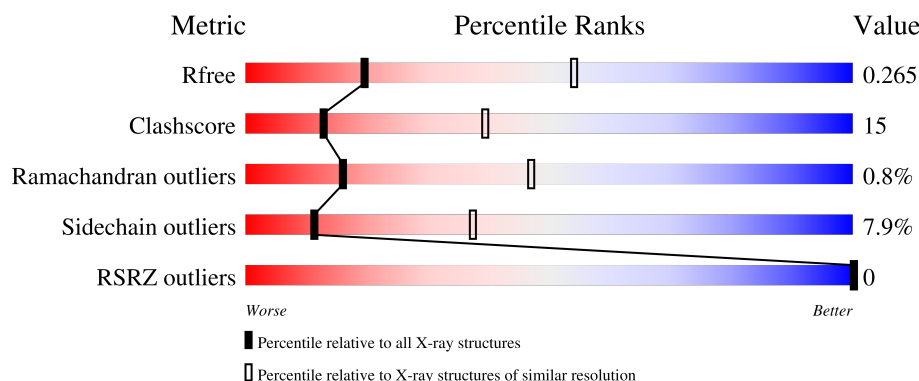
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



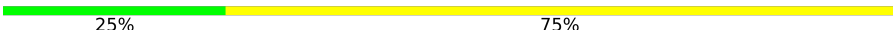
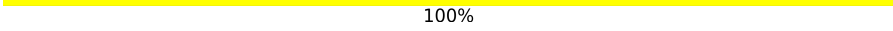
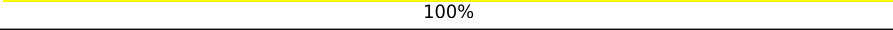
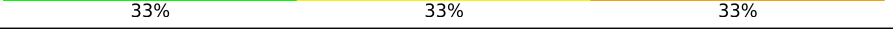
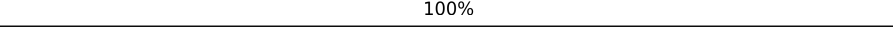
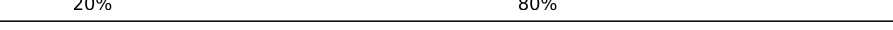
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	966	
1	B	966	
1	C	966	
1	D	966	
2	E	4	

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Mol	Chain	Length	Quality of chain
2	Q	4	 25% 75%
3	F	2	 50% 50%
3	G	2	 50% 50%
3	J	2	 50% 50%
3	K	2	 50% 50%
3	L	2	 50% 50%
3	M	2	 100%
3	P	2	 50% 50%
3	S	2	 100%
4	H	3	 33% 33% 33%
4	I	3	 100%
4	O	3	 67% 33%
4	R	3	 33% 67%
5	N	5	 20% 80%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	BR	C	1008	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 29963 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 Endoplasmic reticulum aminopeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	915	Total	C	N	O	S	0	2	0
			7389	4758	1225	1372	34			
1	B	907	Total	C	N	O	S	0	3	0
			7318	4710	1214	1361	33			
1	C	883	Total	C	N	O	S	0	0	0
			7126	4598	1174	1326	28			
1	D	884	Total	C	N	O	S	0	3	0
			7065	4558	1172	1306	29			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	392	ASN	LYS	variant	UNP Q6P179
A	961	ARG	-	expression tag	UNP Q6P179
A	962	HIS	-	expression tag	UNP Q6P179
A	963	HIS	-	expression tag	UNP Q6P179
A	964	HIS	-	expression tag	UNP Q6P179
A	965	HIS	-	expression tag	UNP Q6P179
A	966	HIS	-	expression tag	UNP Q6P179
B	392	ASN	LYS	variant	UNP Q6P179
B	961	ARG	-	expression tag	UNP Q6P179
B	962	HIS	-	expression tag	UNP Q6P179
B	963	HIS	-	expression tag	UNP Q6P179
B	964	HIS	-	expression tag	UNP Q6P179
B	965	HIS	-	expression tag	UNP Q6P179
B	966	HIS	-	expression tag	UNP Q6P179
C	392	ASN	LYS	variant	UNP Q6P179
C	961	ARG	-	expression tag	UNP Q6P179
C	962	HIS	-	expression tag	UNP Q6P179
C	963	HIS	-	expression tag	UNP Q6P179
C	964	HIS	-	expression tag	UNP Q6P179
C	965	HIS	-	expression tag	UNP Q6P179
C	966	HIS	-	expression tag	UNP Q6P179

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Chain	Residue	Modelled	Actual	Comment	Reference
D	392	ASN	LYS	variant	UNP Q6P179
D	961	ARG	-	expression tag	UNP Q6P179
D	962	HIS	-	expression tag	UNP Q6P179
D	963	HIS	-	expression tag	UNP Q6P179
D	964	HIS	-	expression tag	UNP Q6P179
D	965	HIS	-	expression tag	UNP Q6P179
D	966	HIS	-	expression tag	UNP Q6P179

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	Q	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



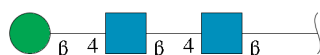
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

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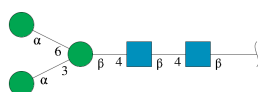
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	S	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	O	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	R	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



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

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

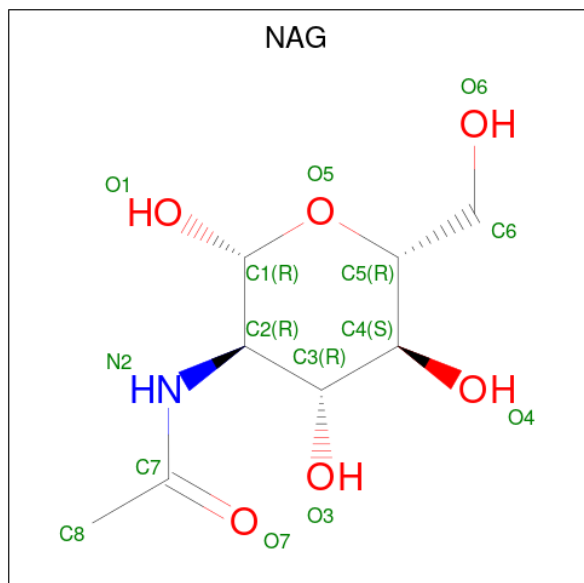
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		
6	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Zn	0	0
			1	1		
6	D	1	Total	Zn	0	0
			1	1		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



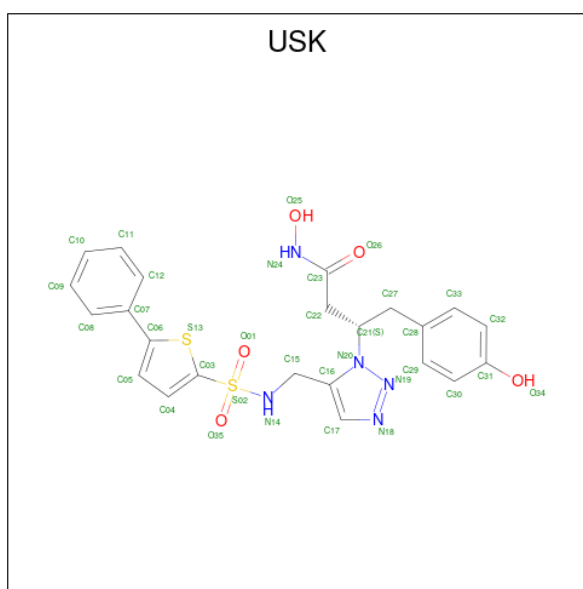
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is (3 {S})-4-(4-hydroxyphenyl)- {N}-oxidanyl-3-[5-[(5-phenylthiophen-2-yl)sulfonylamino]methyl]-1,2,3-triazol-1-yl]butanamide (CCD ID: USK) (formula: C₂₃H₂₃N₅O₅S₂).



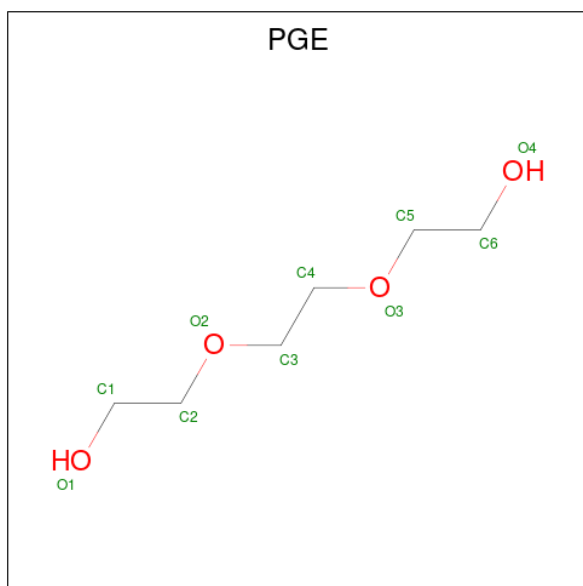
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0	0
			35	23	5	5	2		
8	B	1	Total	C	N	O	S	0	0
			35	23	5	5	2		
8	C	1	Total	C	N	O	S	0	0
			35	23	5	5	2		

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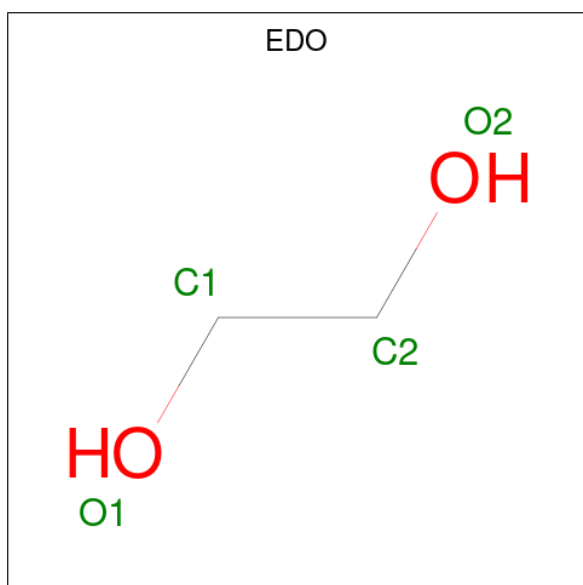
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	D	1	Total	C	N	O	S	0	0
			35	23	5	5	2		

- Molecule 9 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 10 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 4 2 2	0	0
10	B	1	Total C O 4 2 2	0	0
10	D	1	Total C O 4 2 2	0	0

- Molecule 11 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	8	Total Br 8 8	0	0
11	B	2	Total Br 2 2	0	0
11	C	2	Total Br 2 2	0	0
11	D	1	Total Br 1 1	0	0

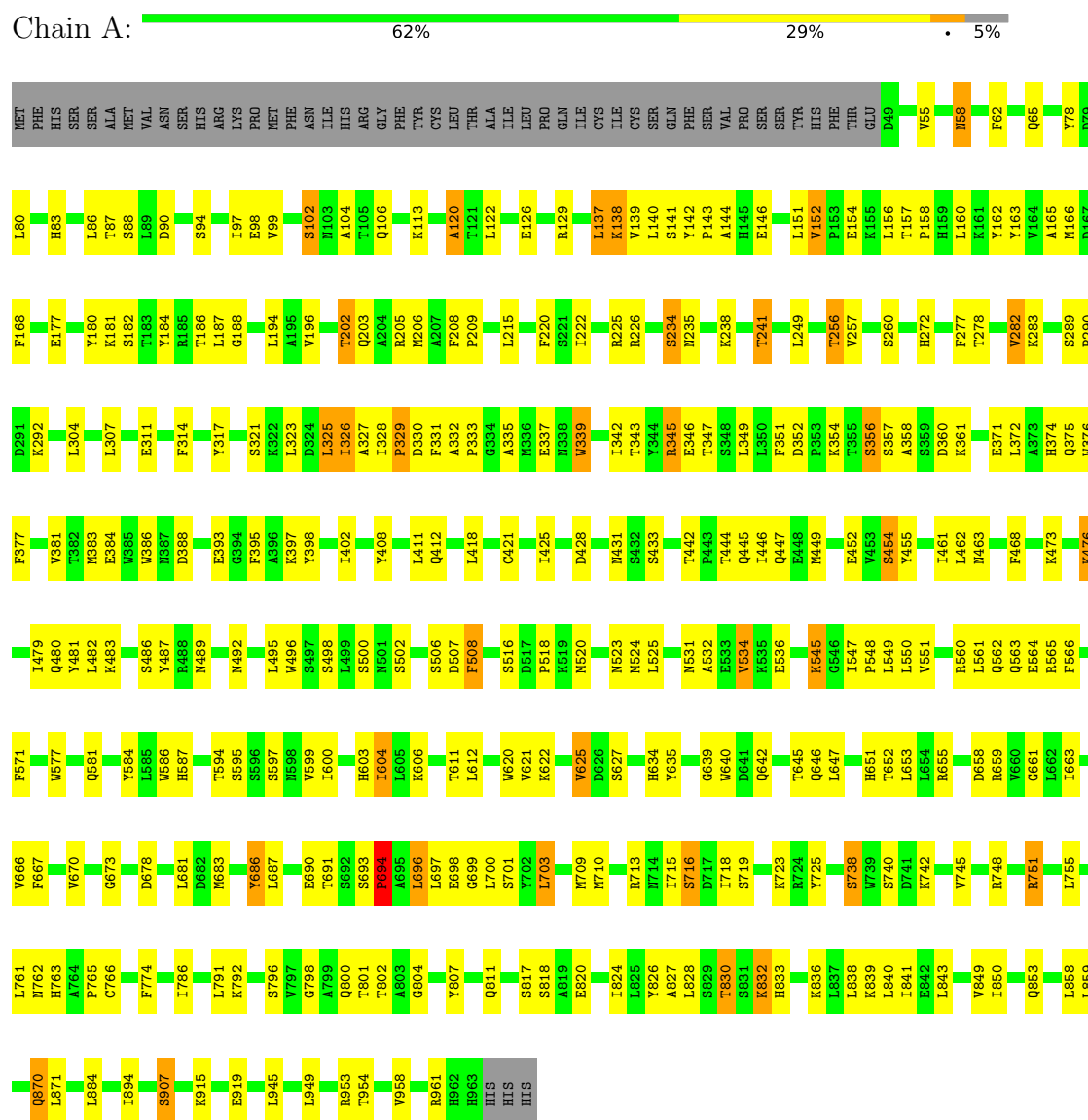
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	39	Total O 39 39	0	0
12	B	37	Total O 37 37	0	0
12	C	21	Total O 21 21	0	0
12	D	10	Total O 10 10	0	0

3 Residue-property plots

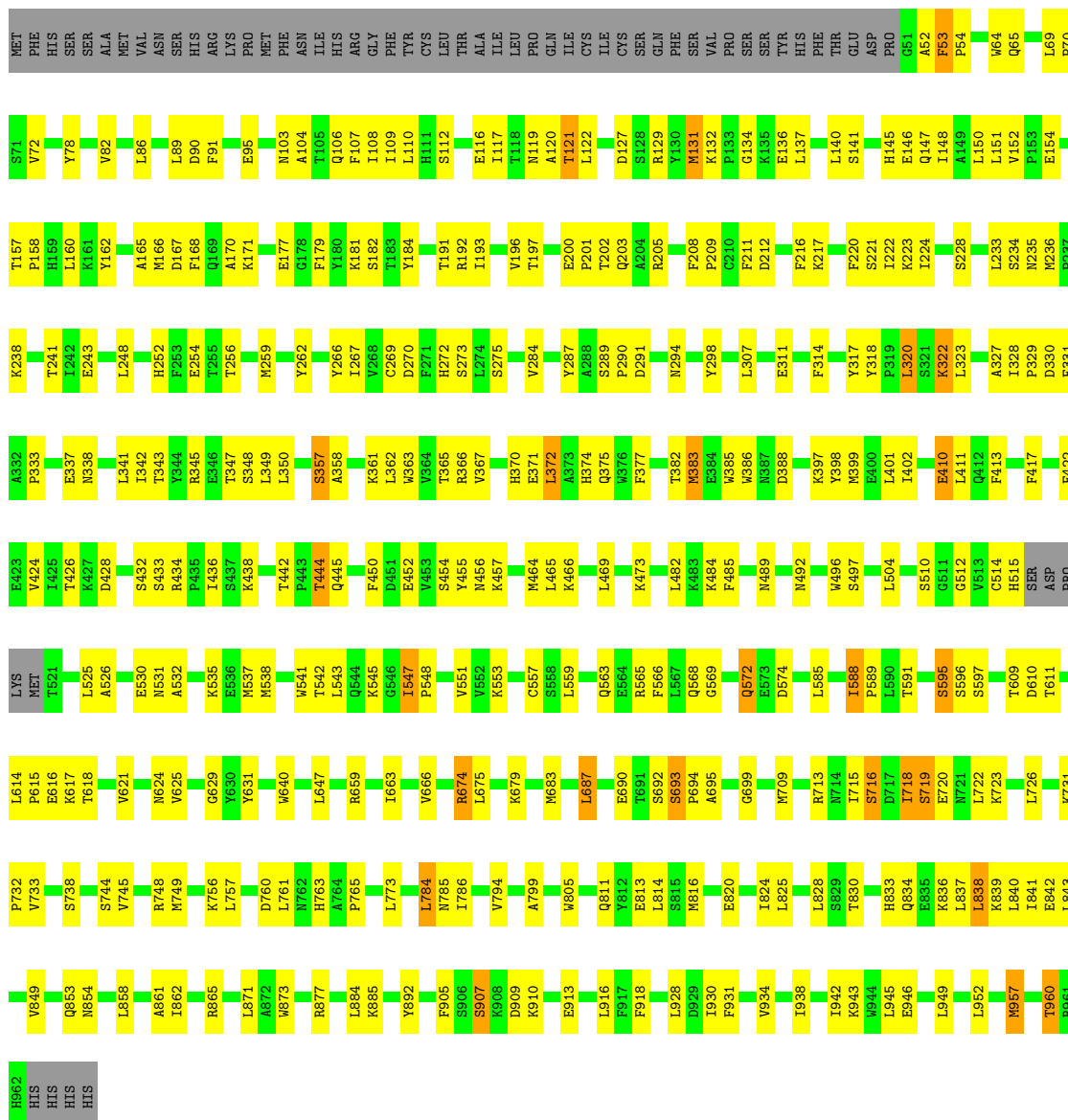
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Endoplasmic reticulum aminopeptidase 2

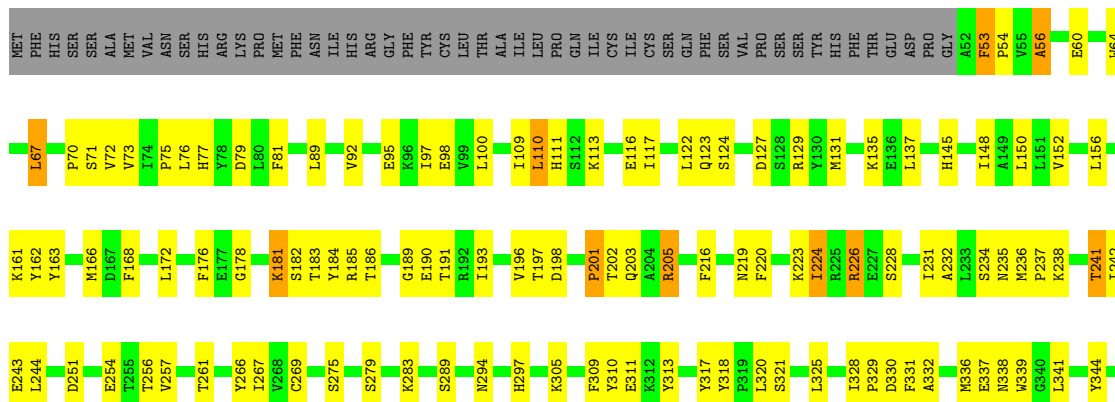


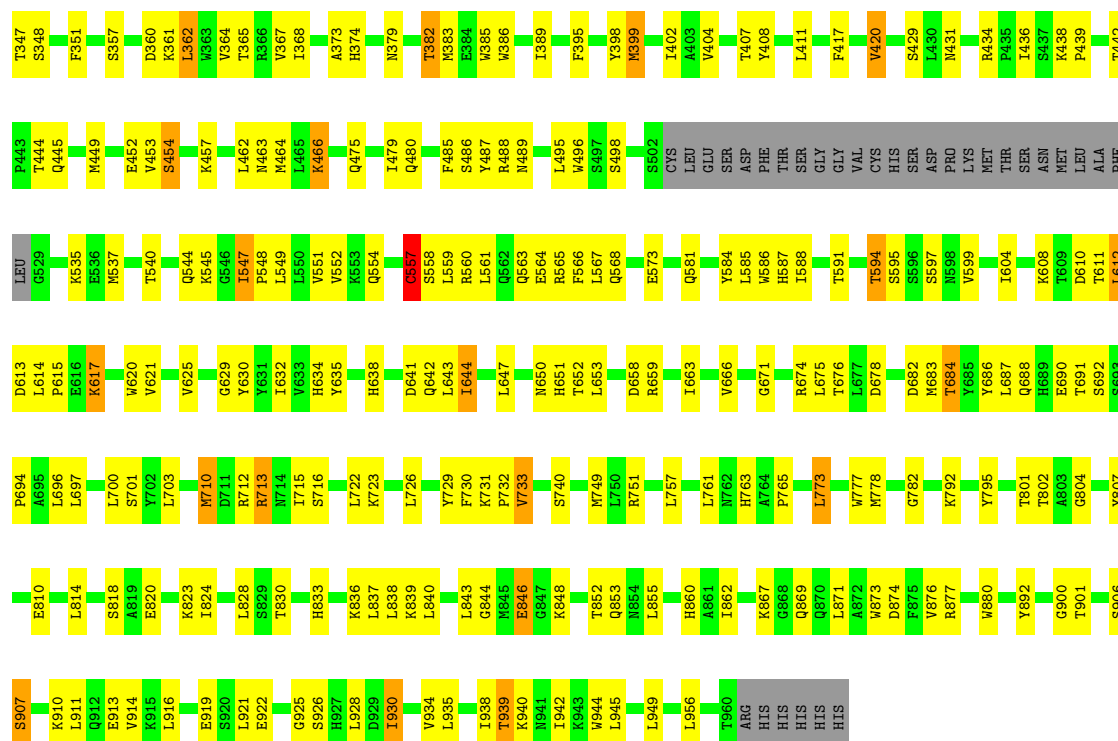
• Molecule 1: Endoplasmic reticulum aminopeptidase 2





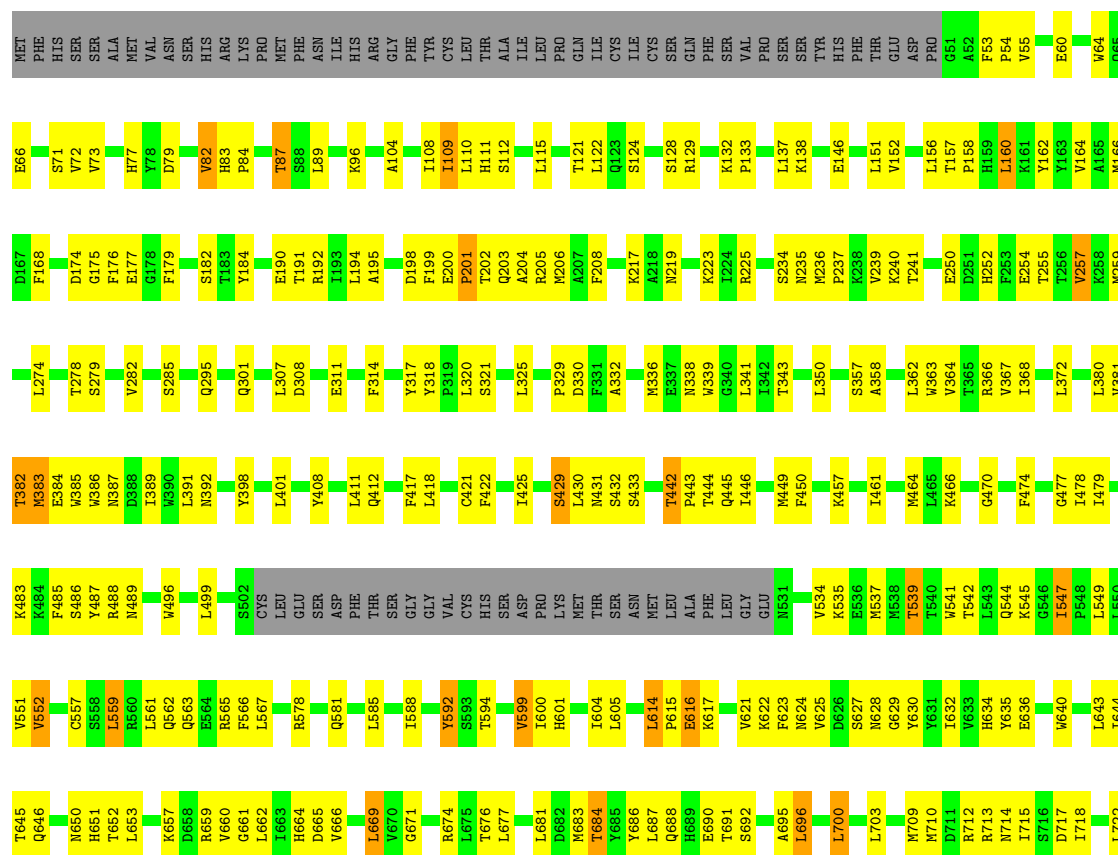
- Molecule 1: Endoplasmic reticulum aminopeptidase 2

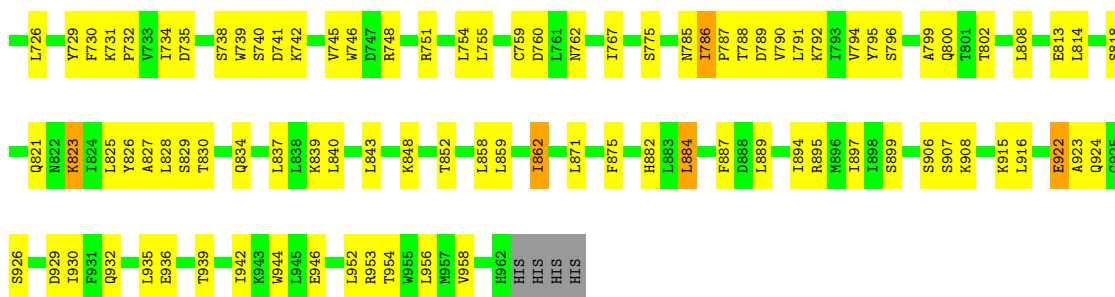




• Molecule 1: Endoplasmic reticulum aminopeptidase 2

Chain D: 55% 34% 8%





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

Chain E: 50% 50%



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

Chain Q: 25% 75%



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

Chain F: 50% 50%



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

Chain G: 50% 50%



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

Chain J: 50% 50%



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

Chain K:  50% 50%

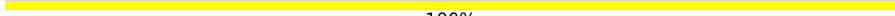


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  50% 50%



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

Chain M:  100%



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

Chain P:  50% 50%



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

Chain S:  100%

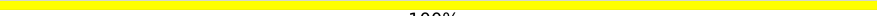


- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  33% 33% 33%



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

Chain I:  100%



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

Chain O:  67% 33%

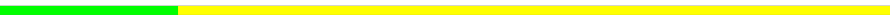
MAG1
MAG2
BMA3

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

Chain R:  33% 67%

MAG1
MAG2
BMA3

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

Chain N:  20% 80%

MAG1
MAG2
BMA3
MAN4
MAN5

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	74.27Å 127.19Å 133.41Å 90.92° 90.08° 90.87°	Depositor
Resolution (Å)	48.66 – 3.10 48.66 – 3.10	Depositor EDS
% Data completeness (in resolution range)	83.2 (48.66-3.10) 79.5 (48.66-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.182 , 0.267 0.183 , 0.265	Depositor DCC
R_{free} test set	3489 reflections (3.94%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 14.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,l,-k 0.000 for h,-l,k 0.013 for h,-k,-l 0.001 for -h,k,-l 0.166 for -h,-k,l 0.000 for -h,l,k 0.000 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	29963	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, PGE, EDO, ZN, NAG, MAN, BR, USK

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	0.47	0/7581	0.69	0/10285
1	B	0.45	0/7507	0.67	2/10185 (0.0%)
1	C	0.41	0/7305	0.62	0/9916
1	D	0.39	0/7252	0.60	0/9862
All	All	0.43	0/29645	0.65	2/40248 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	713	ARG	CA-C-N	-7.22	108.61	122.61
1	B	713	ARG	C-N-CA	-7.22	108.61	122.61

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	557	CYS	Peptide

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	7389	0	7273	213	0
1	B	7318	0	7186	218	0
1	C	7126	0	6990	226	0
1	D	7065	0	6865	237	0
2	E	50	0	43	0	0
2	Q	50	0	43	0	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	1	0
3	L	28	0	25	1	0
3	M	28	0	25	0	0
3	P	28	0	25	0	0
3	S	28	0	25	0	0
4	H	39	0	34	1	0
4	I	39	0	34	0	0
4	O	39	0	34	0	0
4	R	39	0	34	1	0
5	N	61	0	52	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	84	0	78	1	0
7	B	42	0	39	2	0
7	C	56	0	52	0	0
7	D	56	0	52	2	0
8	A	35	0	0	0	0
8	B	35	0	0	2	0
8	C	35	0	0	2	0
8	D	35	0	0	1	0
9	A	10	0	14	0	0
10	A	4	0	6	0	0
10	B	4	0	6	0	0
10	D	4	0	6	0	0
11	A	8	0	0	3	0
11	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	C	2	0	0	4	0
11	D	1	0	0	0	0
12	A	39	0	0	3	0
12	B	37	0	0	11	0
12	C	21	0	0	3	0
12	D	10	0	0	2	0
All	All	29963	0	29041	887	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 15.

All (887) 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:220:PHE:H	1:A:256:THR:HG22	1.14	1.06
1:C:659:ARG:HH12	1:C:691:THR:HG22	1.26	0.97
1:C:362:LEU:CD2	11:C:1008:BR:BR	2.68	0.97
1:B:205:ARG:HH21	1:B:212:ASP:HB3	1.31	0.92
1:C:659:ARG:NH1	1:C:690:GLU:OE2	2.03	0.90
1:A:766[B]:CYS:SG	11:A:1016:BR:BR	2.85	0.90
1:B:563:GLN:HE22	1:B:585:LEU:HA	1.41	0.85
1:A:742:LYS:O	1:A:751:ARG:NH2	2.09	0.84
1:D:600:ILE:HD13	1:D:625:VAL:HG11	1.59	0.84
1:C:945:LEU:HD22	1:C:949:LEU:HD22	1.61	0.83
1:D:425:ILE:O	1:D:429:SER:OG	1.98	0.82
1:A:442:THR:HB	1:A:445:GLN:HG3	1.61	0.82
1:B:510:SER:HA	1:B:515:HIS:HA	1.60	0.81
1:B:382:THR:HG23	1:B:383:MET:HE3	1.65	0.79
1:C:362:LEU:HD21	11:C:1008:BR:BR	2.38	0.79
1:A:723:LYS:HG3	1:A:761:LEU:HB3	1.62	0.79
1:A:220:PHE:H	1:A:256:THR:CG2	1.95	0.77
1:B:122:LEU:HD11	1:B:162:TYR:HB3	1.66	0.77
1:D:278:THR:HG21	1:D:307:LEU:HD23	1.66	0.77
1:C:564:GLU:HB3	1:C:581:GLN:HE21	1.49	0.76
1:B:254:GLU:OE2	12:B:1102:HOH:O	2.03	0.76
1:D:177:GLU:HG2	1:D:203:GLN:HE21	1.52	0.75
7:B:1002:NAG:O3	12:B:1101:HOH:O	2.03	0.75
1:C:224:ILE:HD11	1:C:232:ALA:HB1	1.67	0.74
1:B:591:THR:HG23	1:B:625:VAL:H	1.49	0.74
1:D:122:LEU:HB2	1:D:137:LEU:HD11	1.68	0.74
1:B:424:VAL:HG12	1:B:452:GLU:HB3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:THR:HG22	1:A:444:THR:H	1.50	0.74
1:B:928:LEU:HB2	1:B:930:ILE:HG22	1.68	0.74
1:B:106:GLN:O	12:B:1103:HOH:O	2.06	0.73
1:A:129:ARG:HH11	1:A:154:GLU:HB3	1.53	0.73
1:B:718:ILE:HD11	1:B:952:LEU:HD23	1.70	0.73
1:C:844:GLY:HA3	1:C:855:LEU:HD13	1.71	0.73
1:C:182:SER:OG	1:C:330:ASP:HB2	1.89	0.73
1:C:184:TYR:HB3	1:C:329:PRO:HG2	1.70	0.73
1:B:177:GLU:HB3	1:B:203:GLN:HG2	1.69	0.72
1:C:802:THR:HG23	1:C:836:LYS:HE3	1.71	0.72
1:C:722:LEU:HG	1:C:956:LEU:HD11	1.70	0.72
1:C:846:GLU:HG2	1:C:848:LYS:H	1.53	0.72
1:C:198:ASP:HA	1:C:336:MET:HE1	1.71	0.72
1:D:259:MET:HE2	1:D:339:TRP:HE3	1.53	0.72
1:D:722:LEU:HG	1:D:956:LEU:HD11	1.72	0.72
1:C:563:GLN:HE22	1:C:586:TRP:H	1.34	0.71
1:C:833:HIS:HB2	1:C:836:LYS:HG3	1.72	0.71
1:C:196:VAL:HG23	1:C:267:ILE:HG12	1.71	0.71
1:B:559:LEU:HD11	1:B:614:LEU:HD13	1.70	0.71
1:D:82:VAL:HG23	1:D:84:PRO:HD3	1.73	0.70
1:D:834:GLN:HG3	1:D:871:LEU:HD12	1.72	0.70
1:C:76:LEU:HD11	1:C:100:LEU:HB2	1.74	0.70
1:C:438:LYS:NZ	12:C:1101:HOH:O	2.24	0.70
1:C:635:TYR:HE2	1:C:643:LEU:HD11	1.55	0.70
1:B:813:GLU:OE1	1:D:848:LYS:NZ	2.24	0.70
1:B:535:LYS:N	12:B:1107:HOH:O	2.25	0.70
1:B:318:TYR:HE1	1:B:375:GLN:HE21	1.40	0.69
1:C:72:VAL:HG23	1:C:73:VAL:HG23	1.72	0.69
1:B:545:LYS:HE3	1:B:565:ARG:HH22	1.57	0.69
1:D:225:ARG:HG3	1:D:250:GLU:HG3	1.74	0.69
1:B:52:ALA:O	12:B:1104:HOH:O	2.11	0.68
1:C:554:GLN:HA	1:C:559:LEU:HD23	1.75	0.68
1:D:671:GLY:HA2	1:D:944:TRP:HD1	1.57	0.68
1:D:545:LYS:HE3	1:D:565:ARG:HH22	1.59	0.68
1:B:434:ARG:NH2	1:B:454:SER:OG	2.26	0.68
1:C:828:LEU:HB3	1:C:840:LEU:HD11	1.73	0.68
1:A:716:SER:HA	1:A:719:SER:HB3	1.75	0.68
1:D:791:LEU:HD11	1:D:795:TYR:CZ	2.28	0.68
1:A:594:THR:HG22	1:A:621:VAL:HG13	1.76	0.68
1:A:516:SER:OG	12:A:1101:HOH:O	2.10	0.68
1:D:111:HIS:HB3	1:D:205:ARG:HD3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LYS:HZ1	1:A:139:VAL:H	1.41	0.67
1:C:678:ASP:O	1:C:682:ASP:HB2	1.95	0.67
1:D:470:GLY:O	1:D:474:PHE:N	2.22	0.67
1:D:659:ARG:NH1	1:D:690:GLU:OE2	2.27	0.66
1:A:945:LEU:HD22	1:A:949:LEU:HD12	1.77	0.66
1:C:463:ASN:OD1	1:C:466:LYS:NZ	2.28	0.66
1:C:597:SER:OG	1:C:599:VAL:HG23	1.95	0.66
1:B:234:SER:OG	1:B:235:ASN:N	2.28	0.66
1:D:398:TYR:OH	1:D:466:LYS:HD3	1.96	0.66
1:B:184:TYR:HB3	1:B:329:PRO:HG2	1.78	0.66
1:A:713:ARG:HB2	1:A:715:ILE:HG13	1.78	0.65
1:D:104:ALA:HB2	1:D:158:PRO:HG3	1.78	0.65
1:A:102:SER:O	1:A:158:PRO:HB3	1.96	0.65
1:D:176:PHE:HD2	1:D:332:ALA:HB2	1.60	0.65
1:B:563:GLN:NE2	1:B:585:LEU:HA	2.12	0.65
1:D:201:PRO:HG2	1:D:202:THR:HG23	1.76	0.65
1:D:563:GLN:HE22	1:D:585:LEU:HA	1.62	0.65
1:B:436:ILE:HD11	1:B:457:LYS:HG2	1.79	0.65
1:A:518:PRO:HD2	1:C:535:LYS:HD3	1.78	0.65
1:D:380:LEU:HD11	1:D:487:TYR:CE1	2.32	0.65
1:A:152:VAL:HG11	1:A:156:LEU:HD21	1.78	0.64
1:A:234:SER:OG	1:A:235:ASN:N	2.29	0.64
1:A:481:TYR:CZ	1:A:495:LEU:HD12	2.33	0.64
1:B:331:PHE:N	1:B:853:GLN:OE1	2.30	0.64
1:C:659:ARG:O	1:C:663:ILE:HG13	1.98	0.64
1:B:526:ALA:O	1:B:530:GLU:HG2	1.97	0.64
1:A:532:ALA:HB2	1:C:585:LEU:HD22	1.80	0.64
1:B:337:GLU:HA	1:B:342:ILE:HG23	1.78	0.64
1:A:184:TYR:HB3	1:A:329:PRO:HG2	1.80	0.64
1:A:560:ARG:HA	1:A:611:THR:HG22	1.78	0.64
1:B:383:MET:H	1:B:383:MET:HE2	1.62	0.64
1:D:718:ILE:HG12	1:D:953:ARG:HG3	1.78	0.64
1:A:327:ALA:HB2	1:A:349:LEU:HD23	1.80	0.63
1:B:545:LYS:HE3	1:B:565:ARG:NH2	2.13	0.63
1:C:242:ILE:HG13	1:C:244:LEU:HD21	1.78	0.63
1:B:398:TYR:OH	1:B:466:LYS:HD3	1.97	0.63
1:D:177:GLU:HB3	1:D:203:GLN:HG2	1.79	0.63
1:B:119:ASN:HB2	1:B:167:ASP:HB2	1.81	0.63
1:B:358:ALA:HB2	1:B:748:ARG:CZ	2.29	0.63
1:C:236:MET:SD	1:C:256:THR:HA	2.39	0.62
1:C:338:ASN:HB2	1:C:341:LEU:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:LYS:O	1:C:365:THR:HG22	2.00	0.62
1:C:201:PRO:HD2	1:C:203:GLN:HE22	1.64	0.62
1:C:801:THR:HG23	1:C:804:GLY:H	1.64	0.62
1:B:433:SER:O	1:B:545:LYS:HD2	1.99	0.62
1:A:256:THR:HG23	1:A:257:VAL:O	2.00	0.62
1:B:873:TRP:CE2	1:B:877:ARG:HD2	2.34	0.62
1:A:548:PRO:HB3	1:A:586:TRP:CE3	2.33	0.62
1:C:122:LEU:HD11	1:C:162:TYR:HB3	1.81	0.62
1:A:358:ALA:HB2	1:A:748:ARG:CZ	2.30	0.62
1:B:201:PRO:HD2	1:B:203:GLN:HE22	1.62	0.61
1:D:236:MET:HE3	1:D:237:PRO:HD2	1.81	0.61
1:C:395:PHE:HE2	1:C:495:LEU:HD21	1.65	0.61
1:C:659:ARG:NH1	1:C:691:THR:HG22	2.09	0.61
1:D:785:ASN:ND2	12:D:1101:HOH:O	2.31	0.61
1:D:790:VAL:HG12	1:D:794:VAL:HG23	1.81	0.61
1:C:362:LEU:HD23	11:C:1008:BR:BR	2.55	0.61
1:A:800:GLN:OE1	1:A:830:THR:HG23	2.00	0.61
1:D:622:LYS:NZ	1:D:624:ASN:O	2.33	0.61
1:D:930:ILE:HD12	1:D:930:ILE:H	1.64	0.61
7:A:1002:NAG:H83	7:A:1002:NAG:H3	1.82	0.61
1:C:365:THR:HG21	1:C:411:LEU:HD13	1.81	0.61
1:C:591:THR:HG23	1:C:625:VAL:H	1.66	0.61
1:B:223:LYS:HD2	1:B:252:HIS:CE1	2.36	0.61
1:D:709:MET:HA	1:D:712:ARG:HD2	1.82	0.61
1:A:659:ARG:NH1	1:A:690:GLU:OE2	2.33	0.61
1:D:259:MET:HE2	1:D:339:TRP:CE3	2.34	0.61
1:D:714:ASN:ND2	12:D:1102:HOH:O	2.33	0.61
1:A:186:THR:HG22	1:A:188:GLY:H	1.65	0.60
1:B:53:PHE:HB3	1:B:54:PRO:HD2	1.82	0.60
1:D:592:TYR:HB3	1:D:623:PHE:HA	1.83	0.60
1:B:382:THR:O	1:B:489:ASN:HA	2.01	0.60
1:C:560:ARG:HA	1:C:611:THR:HG22	1.83	0.60
1:C:777:TRP:NE1	1:C:782:GLY:HA2	2.17	0.60
1:D:168:PHE:CE1	1:D:208:PHE:HA	2.36	0.60
1:C:911:LEU:HD11	1:C:939:THR:HG23	1.82	0.60
1:B:366:ARG:HD2	1:B:413:PHE:CE1	2.37	0.60
1:B:547:ILE:HG23	1:B:566:PHE:HB3	1.82	0.60
1:C:442:THR:HB	1:C:445:GLN:HG3	1.83	0.60
1:D:827:ALA:O	1:D:830:THR:HG22	2.01	0.60
1:C:331:PHE:N	1:C:853:GLN:OE1	2.34	0.60
1:A:954:THR:O	1:A:958:VAL:HG23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:945:LEU:HD22	1:B:949:LEU:HD12	1.82	0.59
1:C:644:ILE:HG12	1:C:683:MET:HE3	1.84	0.59
1:D:659:ARG:HH12	1:D:692:SER:HB3	1.67	0.59
1:C:152:VAL:HG11	1:C:156:LEU:HD11	1.85	0.59
1:D:688:GLN:HB2	1:D:729:TYR:CE2	2.38	0.59
1:B:363:TRP:O	1:B:367:VAL:HG23	2.03	0.59
1:A:525:LEU:HD21	1:C:544:GLN:HG2	1.85	0.59
1:C:309:PHE:HZ	1:C:402:ILE:HG22	1.68	0.59
1:D:408:TYR:HB3	1:D:411:LEU:HD12	1.85	0.59
1:A:138:LYS:HB3	1:A:151:LEU:HB2	1.84	0.59
1:A:182:SER:OG	1:A:330:ASP:HB2	2.03	0.58
1:B:327:ALA:HB2	1:B:349:LEU:HD23	1.85	0.58
1:B:873:TRP:CZ2	1:B:877:ARG:HD2	2.38	0.58
1:B:545:LYS:NZ	3:K:1:NAG:O6	2.35	0.58
1:A:337:GLU:HA	1:A:342:ILE:HG12	1.85	0.58
1:C:561:LEU:HD11	1:C:612:LEU:HD12	1.86	0.58
1:D:713:ARG:HH12	1:D:907:SER:HB2	1.68	0.58
1:A:337:GLU:HG3	1:A:374:HIS:HB3	1.85	0.58
1:C:156:LEU:HD23	1:C:162:TYR:CD2	2.38	0.58
1:B:197:THR:HG23	1:B:266:TYR:O	2.04	0.58
1:C:558:SER:HA	1:C:614:LEU:HD21	1.84	0.58
1:C:795:TYR:CD2	1:C:824:ILE:HG12	2.39	0.58
1:D:72:VAL:HG23	1:D:73:VAL:HG23	1.85	0.58
1:B:192:ARG:HA	1:D:190:GLU:HG2	1.86	0.57
1:C:740:SER:O	1:C:751:ARG:NH1	2.37	0.57
1:B:838:LEU:HA	1:B:841:ILE:HG12	1.84	0.57
1:D:687:LEU:HD22	1:D:696:LEU:HA	1.87	0.57
1:A:536:GLU:HG2	1:C:608:LYS:HD2	1.85	0.57
1:B:763:HIS:CD2	1:B:765:PRO:HD2	2.39	0.57
1:C:663:ILE:HG12	1:C:686:TYR:OH	2.03	0.57
1:C:310:TYR:CZ	1:C:373:ALA:HB2	2.39	0.57
1:D:257:VAL:HG12	4:R:1:NAG:H61	1.87	0.57
1:D:433:SER:O	1:D:545:LYS:HD2	2.04	0.57
1:D:599:VAL:HG12	1:D:600:ILE:H	1.70	0.57
1:A:166:MET:HE1	1:A:209:PRO:HB2	1.86	0.57
1:B:942:ILE:O	1:B:946:GLU:HG3	2.04	0.57
1:C:874:ASP:OD1	1:C:877:ARG:NH2	2.36	0.57
1:B:424:VAL:HG11	1:B:456:ASN:HB2	1.86	0.57
1:C:220:PHE:N	1:C:256:THR:OG1	2.29	0.57
7:D:1002:NAG:H3	7:D:1002:NAG:H83	1.85	0.57
1:A:500:SER:OG	1:A:531:ASN:O	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:LYS:HD2	1:A:584:TYR:OH	2.05	0.57
1:D:646:GLN:HE22	1:D:653:LEU:HD12	1.70	0.57
7:D:1005:NAG:H83	7:D:1005:NAG:H3	1.86	0.56
1:A:157:THR:OG1	1:A:160:LEU:HD12	2.05	0.56
1:A:473:LYS:HG2	1:A:502:SER:HB2	1.86	0.56
1:C:713:ARG:HH12	1:C:907:SER:CB	2.18	0.56
1:A:122:LEU:HD11	1:A:162:TYR:HB3	1.88	0.56
1:A:723:LYS:NZ	12:A:1105:HOH:O	2.37	0.56
1:B:127:ASP:OD1	1:B:129:ARG:HD3	2.05	0.56
1:B:820:GLU:O	1:B:824:ILE:HG13	2.05	0.56
1:C:934:VAL:O	1:C:938:ILE:HG13	2.05	0.56
1:D:636:GLU:OE2	1:D:674:ARG:NH1	2.38	0.56
1:A:518:PRO:O	1:C:535:LYS:NZ	2.38	0.56
1:B:337:GLU:HG3	1:B:374:HIS:HB3	1.87	0.56
1:A:345:ARG:HB2	11:A:1015:BR:BR	2.61	0.56
1:B:377:PHE:CE1	1:B:482:LEU:HD21	2.40	0.56
1:A:331:PHE:CE2	1:A:333:PRO:HG2	2.41	0.56
1:B:70:PRO:HD3	1:B:109:ILE:HD11	1.86	0.56
1:C:436:ILE:HD11	1:C:457:LYS:HG2	1.88	0.56
1:A:431:ASN:HA	1:A:565:ARG:HH22	1.71	0.56
1:B:338:ASN:HB2	1:B:341:LEU:O	2.06	0.56
1:B:345:ARG:NH2	1:B:854:ASN:OD1	2.39	0.56
1:D:703:LEU:HD23	1:D:726:LEU:HD21	1.87	0.56
1:D:762:ASN:HA	1:D:767:ILE:HD11	1.88	0.56
1:A:388:ASP:OD1	1:A:492:ASN:HB2	2.05	0.55
1:B:248:LEU:HD22	4:H:1:NAG:H83	1.88	0.55
1:B:526:ALA:O	1:B:530:GLU:N	2.35	0.55
1:B:337:GLU:HB3	1:B:371:GLU:OE2	2.06	0.55
1:C:408:TYR:HB3	1:C:411:LEU:HD12	1.87	0.55
1:A:215:LEU:HA	1:A:489:ASN:ND2	2.22	0.55
1:B:311:GLU:HG2	1:B:317:TYR:HA	1.87	0.55
1:B:318:TYR:CE2	1:B:320:LEU:HB2	2.42	0.55
1:B:569:GLY:O	1:B:943:LYS:HD3	2.07	0.55
1:A:421:CYS:O	1:A:425:ILE:HG13	2.06	0.55
1:B:273:SER:HB3	1:B:287:TYR:CE1	2.41	0.55
1:C:357:SER:HB3	1:C:360:ASP:H	1.71	0.55
1:D:431:ASN:HA	1:D:565:ARG:NH2	2.22	0.55
1:B:723:LYS:HG3	1:B:761:LEU:HB3	1.89	0.55
1:C:183:THR:HG22	1:C:193:ILE:HD13	1.89	0.55
1:C:442:THR:HG22	1:C:444:THR:H	1.71	0.55
1:C:557:CYS:SG	1:C:617:LYS:HA	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:GLU:HG2	1:A:317:TYR:HA	1.88	0.54
1:A:698:GLU:O	1:A:701:SER:N	2.39	0.54
1:B:201:PRO:HG2	1:B:202:THR:HG23	1.89	0.54
1:B:168:PHE:CE2	1:B:208:PHE:HA	2.42	0.54
1:C:79:ASP:O	1:C:95:GLU:HA	2.07	0.54
1:A:738:SER:O	1:A:751:ARG:HD3	2.07	0.54
1:B:905:PHE:HB2	1:B:938:ILE:HD13	1.90	0.54
1:C:449:MET:O	1:C:454:SER:OG	2.24	0.54
1:C:860:HIS:HD2	1:C:900:GLY:HA2	1.72	0.54
1:A:330:ASP:HA	1:A:853:GLN:OE1	2.07	0.54
1:B:182:SER:HB2	1:B:330:ASP:HB3	1.89	0.54
1:B:629:GLY:HA3	1:B:631:TYR:CE1	2.43	0.54
1:C:928:LEU:HB2	1:C:930:ILE:HG22	1.88	0.54
1:C:364:VAL:O	1:C:368:ILE:HG13	2.07	0.54
1:D:664:HIS:ND1	1:D:665:ASP:OD1	2.41	0.54
1:B:107:PHE:HA	12:B:1103:HOH:O	2.07	0.54
1:B:64:TRP:CE2	1:B:70:PRO:HG3	2.43	0.54
1:B:236:MET:HE2	1:B:320:LEU:HD22	1.89	0.54
1:D:364:VAL:O	1:D:368:ILE:HG13	2.08	0.54
1:C:638:HIS:HB3	1:C:641:ASP:HB2	1.90	0.54
1:D:53:PHE:HB3	1:D:54:PRO:HD2	1.90	0.54
1:D:383:MET:SD	1:D:392:ASN:ND2	2.81	0.54
1:D:700:LEU:HD11	1:D:730:PHE:CZ	2.43	0.54
1:B:122:LEU:HB3	1:B:137:LEU:HD11	1.90	0.53
1:B:141:SER:HA	1:B:148:ILE:HG22	1.89	0.53
1:D:234:SER:OG	1:D:235:ASN:N	2.41	0.53
1:C:220:PHE:HZ	1:C:261:THR:HG22	1.73	0.53
1:D:79:ASP:HB2	1:D:96:LYS:HB2	1.91	0.53
1:D:386:TRP:CD1	1:D:446:ILE:HD13	2.43	0.53
1:B:442:THR:HB	1:B:445:GLN:HG3	1.89	0.53
1:B:496:TRP:CZ2	1:B:542:THR:HG21	2.43	0.53
1:B:538:MET:O	1:B:542:THR:HG23	2.08	0.53
1:C:89:LEU:HD22	1:C:181:LYS:HD3	1.91	0.53
1:C:485:PHE:HA	1:C:488:ARG:HD3	1.91	0.53
1:D:199:PHE:HB3	1:D:204:ALA:HB2	1.91	0.53
1:A:215:LEU:HA	1:A:489:ASN:HD21	1.74	0.53
1:C:395:PHE:CD2	1:C:462:LEU:HD11	2.44	0.53
1:C:398:TYR:OH	1:C:466:LYS:HD3	2.08	0.53
1:C:873:TRP:CZ2	1:C:877:ARG:HD3	2.44	0.53
1:D:828:LEU:HB3	1:D:840:LEU:HD11	1.90	0.53
1:A:446:ILE:O	1:A:447:GLN:C	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:SER:HB3	1:A:620:TRP:H	1.73	0.53
1:C:540:THR:HG21	1:C:587:HIS:H	1.73	0.53
1:D:77:HIS:ND1	1:D:219:ASN:HB2	2.24	0.53
1:D:115:LEU:HD13	1:D:168:PHE:CD1	2.43	0.53
3:L:2:NAG:O7	3:L:2:NAG:O3	2.26	0.53
1:B:784:LEU:HD22	1:B:785:ASN:H	1.74	0.53
1:C:243:GLU:O	1:C:244:LEU:HD23	2.09	0.53
1:D:389:ILE:HG21	1:D:449:MET:HB3	1.90	0.53
1:D:450:PHE:O	1:D:895:ARG:NH2	2.35	0.53
1:C:634:HIS:CE1	1:C:675:LEU:HD11	2.44	0.52
1:D:488:ARG:C	1:D:489:ASN:HD22	2.16	0.52
1:B:108:ILE:HB	1:B:150:LEU:HB2	1.90	0.52
1:B:397:LYS:HD3	1:B:455:TYR:HB3	1.91	0.52
1:D:627:SER:OG	1:D:661:GLY:HA3	2.09	0.52
1:D:710:MET:HE1	1:D:718:ILE:HD12	1.91	0.52
1:B:150:LEU:HD11	1:B:166:MET:HE2	1.91	0.52
1:C:910:LYS:HD3	1:C:913:GLU:OE2	2.08	0.52
1:D:138:LYS:HB3	1:D:151:LEU:HB2	1.91	0.52
1:D:839:LYS:O	1:D:843:LEU:HG	2.09	0.52
1:A:325:LEU:N	1:A:325:LEU:HD12	2.25	0.52
1:B:442:THR:HG22	1:B:444:THR:H	1.74	0.52
1:C:77:HIS:ND1	1:C:219:ASN:HB2	2.24	0.52
1:C:475:GLN:O	1:C:479:ILE:HG12	2.09	0.52
1:C:549:LEU:HD12	1:C:632:ILE:O	2.10	0.52
1:C:610:ASP:OD1	1:C:611:THR:N	2.43	0.52
1:C:838:LEU:HD12	1:C:871:LEU:HD11	1.91	0.52
1:D:594:THR:HG22	1:D:621:VAL:HG13	1.92	0.52
1:A:122:LEU:HB2	1:A:137:LEU:HD21	1.91	0.52
1:D:464:MET:HG3	1:D:629:GLY:HA2	1.90	0.52
1:C:763:HIS:CG	1:C:765:PRO:HD2	2.44	0.52
1:C:325:LEU:HD23	1:C:344:TYR:HE2	1.74	0.52
1:A:486:SER:HB3	1:A:487:TYR:CD1	2.45	0.52
1:A:801:THR:HG23	1:A:804:GLY:H	1.75	0.52
1:C:336:MET:HE3	1:C:338:ASN:HD21	1.75	0.52
1:A:571:PHE:CD2	1:A:673:GLY:HA3	2.45	0.51
1:C:666:VAL:HG21	1:C:683:MET:SD	2.49	0.51
1:D:199:PHE:CG	1:D:204:ALA:HA	2.45	0.51
1:D:748:ARG:HB3	1:D:789:ASP:OD2	2.09	0.51
1:A:849:VAL:HG12	1:A:850:ILE:HG13	1.93	0.51
1:A:146:GLU:OE1	1:A:205:ARG:HD2	2.11	0.51
1:A:272:HIS:CE1	1:A:290:PRO:HB3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:LEU:HD22	1:A:696:LEU:HA	1.92	0.51
1:C:67:LEU:HG	1:C:145:HIS:CE1	2.45	0.51
1:C:234:SER:OG	1:C:235:ASN:N	2.44	0.51
1:D:496:TRP:HE1	1:D:542:THR:HG21	1.75	0.51
1:B:839:LYS:O	1:B:843:LEU:HG	2.11	0.51
1:B:873:TRP:O	1:B:877:ARG:HD3	2.09	0.51
1:C:676:THR:OG1	1:C:678:ASP:OD1	2.19	0.51
1:D:825:LEU:HD11	1:D:858:LEU:HD13	1.91	0.51
1:D:182:SER:OG	1:D:330:ASP:HB3	2.10	0.51
1:D:614:LEU:HD21	1:D:617:LYS:H	1.75	0.51
1:D:887:PHE:HB2	1:D:894:ILE:HG12	1.93	0.51
1:B:834:GLN:HB3	1:B:871:LEU:HD12	1.93	0.51
1:C:176:PHE:HD2	1:C:332:ALA:HB2	1.74	0.51
1:C:313:TYR:CE2	1:C:399:MET:HE1	2.45	0.51
1:B:382:THR:HG23	1:B:383:MET:CE	2.36	0.51
1:B:830:THR:HG23	1:B:865:ARG:NH2	2.26	0.51
1:D:431:ASN:O	1:D:545:LYS:NZ	2.44	0.51
1:D:734:ILE:HG12	1:D:754:LEU:HD22	1.93	0.51
1:C:116:GLU:O	1:C:168:PHE:HA	2.10	0.51
1:C:431:ASN:HA	1:C:565:ARG:NH2	2.26	0.51
1:D:128:SER:O	1:D:129:ARG:HG2	2.11	0.51
1:D:740:SER:HA	1:D:787:PRO:HG2	1.94	0.50
1:A:603:HIS:CE1	1:A:612:LEU:HD21	2.47	0.50
1:C:113:LYS:NZ	12:C:1106:HOH:O	2.44	0.50
1:D:199:PHE:CD1	1:D:204:ALA:HA	2.47	0.50
1:A:683:MET:O	1:A:686:TYR:HD2	1.94	0.50
1:D:338:ASN:HB2	1:D:341:LEU:O	2.11	0.50
1:D:731:LYS:N	1:D:732:PRO:HD2	2.26	0.50
1:C:226:ARG:HD3	1:C:251:ASP:OD2	2.12	0.50
1:C:417:PHE:O	1:C:420:VAL:HG22	2.11	0.50
1:D:152:VAL:HG11	1:D:156:LEU:HD11	1.93	0.50
1:B:121:THR:HG22	7:B:1004:NAG:H82	1.94	0.50
1:B:235:ASN:O	1:B:322:LYS:HE3	2.11	0.50
1:D:442:THR:HG22	1:D:443:PRO:HD2	1.94	0.50
1:D:671:GLY:HA2	1:D:944:TRP:CD1	2.43	0.50
1:A:622:LYS:NZ	1:A:658:ASP:OD1	2.44	0.50
1:A:800:GLN:HE22	1:A:832:LYS:HD3	1.77	0.50
1:B:145:HIS:O	1:B:147:GLN:HG3	2.12	0.50
1:B:236:MET:SD	1:B:256:THR:HA	2.51	0.50
1:C:650:ASN:HB3	1:C:653:LEU:HG	1.94	0.50
1:C:348:SER:HB3	1:C:367:VAL:HG11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:401:LEU:HD13	1:D:417:PHE:HB2	1.94	0.49
1:D:634:HIS:HB2	1:D:669:LEU:HD11	1.94	0.49
1:B:745:VAL:HG12	1:B:749:MET:HE3	1.94	0.49
1:D:87:THR:O	1:D:89:LEU:HG	2.12	0.49
1:A:339:TRP:HA	1:A:375:GLN:HE22	1.77	0.49
1:A:840:LEU:HB3	1:A:858:LEU:HD21	1.93	0.49
1:B:374:HIS:HA	1:B:377:PHE:O	2.12	0.49
1:C:683:MET:O	1:C:686:TYR:HD1	1.94	0.49
1:A:412:GLN:OE1	1:A:745:VAL:HB	2.12	0.49
1:A:627:SER:OG	1:A:661:GLY:HA3	2.13	0.49
1:A:796:SER:HB3	1:A:827:ALA:HA	1.95	0.49
1:D:217:LYS:HE3	1:D:489:ASN:HD21	1.77	0.49
1:D:311:GLU:HG2	1:D:317:TYR:HA	1.95	0.49
1:A:226:ARG:NH2	1:A:249:LEU:HD22	2.27	0.49
1:B:64:TRP:CZ2	1:B:70:PRO:HG3	2.47	0.49
1:B:314:PHE:CE1	1:B:399:MET:HE2	2.48	0.49
1:B:726:LEU:HD13	1:B:757:LEU:HD11	1.95	0.49
1:D:604:ILE:HD12	1:D:604:ILE:H	1.76	0.49
1:A:506:SER:O	1:A:508:PHE:N	2.45	0.49
1:A:802:THR:HG22	1:A:836:LYS:HE3	1.94	0.49
1:A:828:LEU:HB3	1:A:840:LEU:HD11	1.94	0.49
1:C:547:ILE:HG13	1:C:548:PRO:HD2	1.94	0.49
1:C:635:TYR:CE2	1:C:643:LEU:HD11	2.42	0.49
1:D:411:LEU:HA	1:D:745:VAL:HG21	1.93	0.49
1:B:690:GLU:HG2	1:B:695:ALA:HB3	1.94	0.49
1:C:568:GLN:HB3	1:C:940:LYS:HZ3	1.78	0.49
1:C:876:VAL:HG21	1:C:901:THR:HG21	1.95	0.49
1:D:362:LEU:O	1:D:362:LEU:HD12	2.12	0.49
1:D:792:LYS:HE3	1:D:823:LYS:HG3	1.94	0.49
1:A:393:GLU:HB3	1:A:455:TYR:CE2	2.48	0.49
1:A:713:ARG:O	1:A:715:ILE:N	2.42	0.49
1:C:137:LEU:HD22	1:C:150:LEU:HB3	1.95	0.49
1:D:622:LYS:HD3	1:D:662:LEU:HD21	1.94	0.49
1:D:651:HIS:NE2	1:D:691:THR:HG22	2.28	0.49
1:D:713:ARG:HD2	1:D:906:SER:OG	2.12	0.49
1:A:565:ARG:HD2	1:A:584:TYR:CD2	2.48	0.49
1:A:687:LEU:HD11	1:A:699:GLY:HA3	1.94	0.49
1:C:837:LEU:HD22	1:C:862:ILE:HD13	1.95	0.49
1:A:792:LYS:HG2	1:A:826:TYR:CD2	2.47	0.49
1:B:370:HIS:C	1:B:370:HIS:CD2	2.92	0.48
1:C:178:GLY:O	1:C:197:THR:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:LYS:HA	1:D:164:VAL:O	2.12	0.48
1:D:421:CYS:O	1:D:425:ILE:HG13	2.12	0.48
1:A:138:LYS:NZ	1:A:139:VAL:H	2.10	0.48
1:A:647:LEU:HD21	1:A:659:ARG:HG2	1.94	0.48
1:B:90:ASP:HA	1:B:171:LYS:HA	1.95	0.48
1:C:594:THR:OG1	1:C:595:SER:N	2.44	0.48
1:A:88:SER:HB3	1:A:90:ASP:OD2	2.13	0.48
1:B:537:MET:HE1	1:B:589:PRO:HB3	1.94	0.48
1:B:715:ILE:O	1:B:719:SER:HB3	2.14	0.48
1:B:786:ILE:HD13	1:B:794:VAL:HG11	1.96	0.48
1:C:687:LEU:HD22	1:C:696:LEU:HA	1.94	0.48
1:D:176:PHE:CD2	1:D:332:ALA:HB2	2.44	0.48
1:A:326:ILE:HG23	1:A:343:THR:HG22	1.95	0.48
1:B:238:LYS:HD2	1:B:241:THR:OG1	2.13	0.48
1:C:242:ILE:HG13	1:C:244:LEU:CD2	2.42	0.48
1:D:547:ILE:HG23	1:D:566:PHE:HB3	1.94	0.48
1:A:104:ALA:HB2	1:A:158:PRO:HD3	1.95	0.48
1:A:655:ARG:O	1:A:658:ASP:N	2.38	0.48
1:B:805:TRP:CE3	1:B:836:LYS:HD3	2.49	0.48
1:C:620:TRP:HB3	1:C:642:GLN:HG2	1.95	0.48
1:C:684:THR:CG2	1:C:703:LEU:HD11	2.43	0.48
1:D:559:LEU:HD21	1:D:621:VAL:HG21	1.95	0.48
1:A:78:TYR:HB2	1:A:220:PHE:CD2	2.49	0.48
1:A:431:ASN:HA	1:A:565:ARG:NH2	2.28	0.48
1:B:647:LEU:HD13	1:B:683:MET:HE2	1.95	0.48
1:D:535:LYS:O	1:D:539:THR:OG1	2.31	0.48
1:D:662:LEU:O	1:D:666:VAL:HG23	2.13	0.48
1:C:122:LEU:HB2	1:C:137:LEU:HD11	1.95	0.48
1:C:336:MET:HE3	1:C:338:ASN:ND2	2.29	0.48
1:D:660:VAL:HG12	1:D:695:ALA:CA	2.44	0.48
1:C:75:PRO:HD2	1:C:216:PHE:HD2	1.79	0.48
1:C:692:SER:HB3	1:C:694:PRO:HD2	1.96	0.48
1:D:362:LEU:O	1:D:366:ARG:HG3	2.14	0.48
1:D:483:LYS:HA	1:D:486:SER:OG	2.13	0.48
1:D:592:TYR:HE1	1:D:601:HIS:HB2	1.79	0.48
1:D:713:ARG:NH1	1:D:907:SER:HB2	2.28	0.48
1:A:203:GLN:HG3	1:A:206:MET:CE	2.44	0.48
1:B:496:TRP:HZ2	1:B:542:THR:HG21	1.78	0.48
1:D:592:TYR:CB	1:D:623:PHE:HA	2.43	0.48
1:D:908:LYS:HG2	1:D:942:ILE:HG21	1.96	0.48
1:A:520:MET:SD	1:C:496:TRP:HD1	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:961:ARG:NH1	1:B:320:LEU:O	2.45	0.47
1:C:236:MET:HE2	1:C:254:GLU:HB3	1.94	0.47
1:C:438:LYS:HG2	1:C:439:PRO:HD2	1.96	0.47
1:D:681:LEU:O	1:D:684:THR:HB	2.14	0.47
1:A:80:LEU:HD23	1:A:222:ILE:HD12	1.95	0.47
1:A:693:SER:HB2	1:A:694:PRO:HD3	1.96	0.47
1:C:389:ILE:HG21	1:C:449:MET:HB3	1.96	0.47
1:C:795:TYR:HD2	1:C:824:ILE:HG12	1.79	0.47
1:A:238:LYS:HD2	1:A:241:THR:HG22	1.96	0.47
1:C:839:LYS:O	1:C:843:LEU:HG	2.15	0.47
1:A:83:HIS:CG	1:A:225:ARG:HD2	2.49	0.47
1:C:365:THR:HG21	1:C:411:LEU:CD1	2.45	0.47
1:B:132:LYS:H	1:B:132:LYS:HD2	1.80	0.47
1:B:833:HIS:HB2	1:B:836:LYS:HG3	1.96	0.47
1:C:651:HIS:HE1	1:C:691:THR:HB	1.80	0.47
1:A:196:VAL:HG21	1:A:328:ILE:CD1	2.45	0.47
1:A:476:LYS:O	1:A:480:GLN:HG2	2.15	0.47
1:A:496:TRP:O	1:A:500:SER:HB2	2.14	0.47
1:A:807:TYR:O	1:A:811:GLN:HG2	2.14	0.47
1:B:398:TYR:CE2	1:B:402:ILE:HD11	2.49	0.47
1:B:464:MET:HE1	1:B:541:TRP:CE2	2.49	0.47
1:C:778:MET:HG3	1:C:807:TYR:CD2	2.49	0.47
1:D:157:THR:OG1	1:D:160:LEU:HD13	2.14	0.47
1:D:198:ASP:OD1	1:D:336:MET:HG2	2.15	0.47
1:C:385:TRP:CG	1:C:386:TRP:N	2.82	0.47
1:D:942:ILE:O	1:D:946:GLU:HG3	2.15	0.47
1:A:106:GLN:O	1:A:152:VAL:HG23	2.15	0.47
1:A:604:ILE:HG22	1:A:606:LYS:HG3	1.95	0.47
1:A:774:PHE:CE1	1:A:798:GLY:HA3	2.50	0.47
1:B:157:THR:OG1	1:B:160:LEU:HD22	2.15	0.47
1:C:584:TYR:HB3	1:C:586:TRP:CZ3	2.50	0.47
1:D:430:LEU:HB3	1:D:936:GLU:OE2	2.15	0.47
1:D:738:SER:HB3	1:D:751:ARG:NH1	2.30	0.47
1:A:386:TRP:CD1	1:A:446:ILE:HD13	2.50	0.47
1:A:560:ARG:HE	1:A:611:THR:HG21	1.78	0.47
1:B:640:TRP:CZ3	1:B:666:VAL:HG12	2.50	0.47
1:C:683:MET:HG3	1:C:686:TYR:HE1	1.80	0.47
1:D:418:LEU:HD23	1:D:418:LEU:HA	1.69	0.47
1:D:792:LYS:HB2	1:D:823:LYS:HG2	1.97	0.47
1:A:226:ARG:HH22	1:A:249:LEU:HD22	1.80	0.46
1:A:314:PHE:O	1:A:479:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:SER:O	1:A:545:LYS:HE2	2.15	0.46
1:B:272:HIS:CD2	1:B:290:PRO:HB3	2.50	0.46
1:B:756:LYS:NZ	1:B:760:ASP:OD2	2.49	0.46
1:B:892:TYR:HB2	8:B:1005:USK:C32	2.45	0.46
1:C:238:LYS:HD2	1:C:241:THR:CG2	2.45	0.46
1:C:362:LEU:HD22	11:C:1008:BR:BR	2.65	0.46
1:C:486:SER:HB3	1:C:487:TYR:HD1	1.80	0.46
1:D:731:LYS:HE3	1:D:735:ASP:OD1	2.15	0.46
1:A:142:TYR:CE1	1:A:144:ALA:HB3	2.50	0.46
1:A:545:LYS:HD3	1:A:565:ARG:NH2	2.30	0.46
1:A:839:LYS:O	1:A:843:LEU:HG	2.15	0.46
1:C:98:GLU:OE2	1:C:161:LYS:HD3	2.16	0.46
1:C:185:ARG:HA	1:C:190:GLU:O	2.15	0.46
1:D:184:TYR:O	1:D:191:THR:HA	2.14	0.46
1:D:442:THR:HB	1:D:445:GLN:H	1.80	0.46
1:D:742:LYS:O	1:D:751:ARG:NH2	2.40	0.46
1:A:323:LEU:HD11	1:A:342:ILE:HD12	1.97	0.46
1:A:449:MET:O	1:A:454:SER:OG	2.31	0.46
1:A:709:MET:HE2	1:A:945:LEU:HG	1.96	0.46
1:B:146:GLU:OE1	1:B:205:ARG:HD2	2.15	0.46
1:B:331:PHE:CE2	1:B:333:PRO:HG2	2.50	0.46
1:B:716:SER:O	1:B:720:GLU:N	2.36	0.46
1:D:158:PRO:O	1:D:160:LEU:HD12	2.15	0.46
1:D:594:THR:OG1	1:D:616:GLU:OE1	2.30	0.46
1:A:120:ALA:HA	1:A:165:ALA:O	2.15	0.46
1:A:398:TYR:CE1	1:A:463:ASN:HB2	2.51	0.46
1:A:600:ILE:HD12	1:A:625:VAL:HG11	1.97	0.46
1:B:168:PHE:CE2	1:B:209:PRO:HD3	2.50	0.46
1:B:179:PHE:CE2	1:B:266:TYR:HE2	2.34	0.46
1:C:339:TRP:CD2	1:C:379:ASN:HB3	2.50	0.46
1:C:548:PRO:HB3	1:C:586:TRP:CD2	2.51	0.46
1:C:938:ILE:O	1:C:942:ILE:HG13	2.16	0.46
1:D:60:GLU:OE1	1:D:138:LYS:NZ	2.35	0.46
1:D:549:LEU:HB2	1:D:566:PHE:HD2	1.81	0.46
1:A:418:LEU:HD11	1:A:627:SER:HB2	1.97	0.46
1:A:681:LEU:HD23	1:A:681:LEU:HA	1.70	0.46
1:C:683:MET:O	1:C:686:TYR:CD1	2.68	0.46
1:A:196:VAL:HG21	1:A:328:ILE:HD13	1.96	0.46
1:A:549:LEU:HB2	1:A:566:PHE:HB2	1.97	0.46
1:B:91:PHE:CE1	1:B:170:ALA:HB3	2.50	0.46
1:C:337:GLU:O	1:C:338:ASN:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:545:LYS:HE3	1:D:565:ARG:NH2	2.28	0.46
1:D:696:LEU:HD12	1:D:700:LEU:HD13	1.97	0.46
1:A:565:ARG:N	1:A:581:GLN:OE1	2.47	0.46
1:B:154:GLU:HA	1:B:154:GLU:OE1	2.16	0.46
1:B:385:TRP:CG	1:B:386:TRP:N	2.84	0.46
1:B:610:ASP:OD1	1:B:611:THR:N	2.47	0.46
1:C:442:THR:HB	1:C:445:GLN:CG	2.46	0.46
1:C:548:PRO:HB3	1:C:586:TRP:CE3	2.51	0.46
1:B:196:VAL:HG23	1:B:267:ILE:HG12	1.97	0.46
1:A:277:PHE:CZ	1:A:283:LYS:HG3	2.51	0.46
1:A:796:SER:HB2	1:A:830:THR:HG21	1.97	0.46
1:A:817:SER:O	1:A:820:GLU:N	2.49	0.46
1:B:411:LEU:HD23	1:B:411:LEU:HA	1.69	0.46
1:B:531:ASN:ND2	12:B:1113:HOH:O	2.48	0.46
1:C:95:GLU:OE1	1:C:166:MET:HE3	2.16	0.46
1:D:146:GLU:OE1	1:D:205:ARG:NH1	2.49	0.46
1:D:634:HIS:NE2	1:D:636:GLU:HG2	2.31	0.46
1:D:657:LYS:O	1:D:660:VAL:HG22	2.16	0.46
1:A:166:MET:HE3	1:A:166:MET:HB2	1.70	0.45
1:A:203:GLN:HG3	1:A:206:MET:HE1	1.98	0.45
1:A:339:TRP:HD1	1:A:375:GLN:NE2	2.14	0.45
1:B:223:LYS:HG2	1:B:252:HIS:HA	1.96	0.45
1:B:675:LEU:HD23	1:B:675:LEU:HA	1.71	0.45
1:A:78:TYR:CD2	1:A:97:ILE:HG12	2.51	0.45
1:A:331:PHE:HB3	1:A:345:ARG:HB3	1.98	0.45
1:B:53:PHE:HB3	1:B:54:PRO:CD	2.47	0.45
1:B:557:CYS:HA	1:B:614:LEU:HD23	1.97	0.45
1:B:687:LEU:HD11	1:B:699:GLY:HA3	1.98	0.45
1:B:816:MET:HA	1:B:816:MET:HE2	1.99	0.45
1:C:713:ARG:HH12	1:C:907:SER:HB3	1.80	0.45
1:B:223:LYS:NZ	12:B:1114:HOH:O	2.49	0.45
1:C:135:LYS:HD2	1:C:135:LYS:HA	1.72	0.45
1:D:174:ASP:OD1	1:D:175:GLY:N	2.49	0.45
1:A:473:LYS:HG2	1:A:502:SER:CB	2.47	0.45
1:B:120:ALA:O	1:B:137:LEU:N	2.44	0.45
1:B:591:THR:O	1:B:624:ASN:N	2.49	0.45
1:B:811:GLN:HA	1:B:814:LEU:HD12	1.98	0.45
1:C:382:THR:O	1:C:489:ASN:HA	2.16	0.45
1:C:880:TRP:CZ2	1:C:921:LEU:HD13	2.52	0.45
1:D:382:THR:O	1:D:489:ASN:HA	2.16	0.45
1:D:464:MET:HE1	1:D:541:TRP:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:751:ARG:HG3	1:D:755:LEU:HD12	1.98	0.45
1:A:351:PHE:CE1	1:A:361:LYS:HB2	2.52	0.45
1:A:461:ILE:HG13	1:A:462:LEU:N	2.32	0.45
1:B:112:SER:HB3	1:B:148:ILE:HG12	1.99	0.45
1:D:683:MET:O	1:D:686:TYR:HD1	1.99	0.45
1:A:635:TYR:HB3	1:A:639:GLY:HA3	1.99	0.45
1:B:909:ASP:O	1:B:913:GLU:HG3	2.16	0.45
1:C:464:MET:HG3	1:C:629:GLY:HA2	1.99	0.45
1:C:547:ILE:HD12	1:C:630:TYR:CD2	2.51	0.45
1:C:749:MET:HB2	1:C:749:MET:HE3	1.75	0.45
1:D:115:LEU:HD13	1:D:168:PHE:HD1	1.81	0.45
1:D:166:MET:HE2	1:D:166:MET:HB3	1.79	0.45
1:D:385:TRP:CD1	1:D:387:ASN:H	2.35	0.45
1:D:551:VAL:CG1	1:D:636:GLU:HG3	2.46	0.45
1:D:935:LEU:O	1:D:939:THR:HG23	2.17	0.45
1:D:592:TYR:CE1	1:D:601:HIS:HB2	2.52	0.45
1:B:78:TYR:HB2	1:B:220:PHE:CD1	2.51	0.45
1:C:183:THR:HB	1:C:191:THR:HG23	1.98	0.45
1:D:363:TRP:O	1:D:367:VAL:HG12	2.17	0.45
1:D:643:LEU:HA	1:D:646:GLN:HB3	1.99	0.45
1:D:922:GLU:O	1:D:924:GLN:N	2.47	0.45
1:A:642:GLN:O	1:A:645:THR:HB	2.17	0.45
1:A:120:ALA:HB2	1:A:166:MET:HG2	1.99	0.45
1:C:540:THR:HG23	1:C:586:TRP:HA	1.99	0.45
1:B:193:ILE:HG13	1:D:190:GLU:HG3	1.99	0.44
1:C:196:VAL:HG22	1:C:197:THR:H	1.81	0.44
1:C:730:PHE:HB3	1:C:733:VAL:HG12	1.98	0.44
1:D:77:HIS:NE2	1:D:79:ASP:OD1	2.48	0.44
1:A:238:LYS:HD2	1:A:241:THR:CG2	2.47	0.44
1:A:520:MET:SD	1:C:496:TRP:CD1	3.10	0.44
1:A:703:LEU:HD21	1:A:725:TYR:HE2	1.82	0.44
1:C:311:GLU:HG2	1:C:317:TYR:HA	1.98	0.44
1:C:408:TYR:CB	1:C:411:LEU:HD12	2.48	0.44
1:C:763:HIS:CE1	1:C:765:PRO:HG2	2.52	0.44
1:D:282:VAL:HG21	1:D:318:TYR:CE2	2.52	0.44
1:D:677:LEU:HD21	1:D:952:LEU:HD13	1.97	0.44
1:A:180:TYR:HD1	1:A:181:LYS:O	1.99	0.44
1:D:200:GLU:HA	1:D:201:PRO:HA	1.75	0.44
1:A:696:LEU:O	1:A:700:LEU:HB2	2.18	0.44
1:B:269:CYS:SG	1:B:270:ASP:N	2.91	0.44
1:B:843:LEU:HD22	1:B:849:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:684:THR:HG21	1:C:703:LEU:HD11	1.99	0.44
1:A:140:LEU:HD11	1:A:151:LEU:HD11	1.99	0.44
1:A:141:SER:O	1:A:143:PRO:HD3	2.18	0.44
1:A:634:HIS:CD2	1:A:640:TRP:HE1	2.34	0.44
1:B:129:ARG:HH12	1:B:157:THR:HG23	1.83	0.44
1:B:572:GLN:HE21	1:B:572:GLN:HB2	1.64	0.44
1:C:81:PHE:HA	1:C:223:LYS:O	2.17	0.44
1:D:115:LEU:HD21	1:D:206:MET:O	2.18	0.44
1:A:425:ILE:HG23	1:A:547:ILE:HD13	2.00	0.44
1:B:422:PHE:O	1:B:426:THR:HG23	2.17	0.44
1:B:731:LYS:N	1:B:732:PRO:HD2	2.33	0.44
1:C:730:PHE:O	1:C:733:VAL:HG12	2.18	0.44
1:C:837:LEU:HD22	1:C:862:ILE:CD1	2.46	0.44
1:D:474:PHE:CE1	1:D:478:ILE:HD11	2.52	0.44
1:B:72:VAL:HG12	1:B:103:ASN:HB2	2.00	0.44
1:B:357:SER:OG	1:B:358:ALA:N	2.51	0.44
1:C:111:HIS:HB3	1:C:205:ARG:HB3	1.99	0.44
1:C:453:VAL:HG13	1:C:457:LYS:HD3	1.99	0.44
1:C:792:LYS:HG3	1:C:823:LYS:HD3	1.99	0.44
1:D:239:VAL:HG23	1:D:240:LYS:N	2.33	0.44
1:D:381:VAL:HG12	1:D:485:PHE:O	2.17	0.44
1:A:357:SER:HB3	1:A:360:ASP:CG	2.42	0.44
1:A:564:GLU:HB2	1:A:581:GLN:OE1	2.17	0.44
1:B:383:MET:O	1:B:383:MET:HG2	2.15	0.44
1:B:438:LYS:HE2	1:B:438:LYS:HB3	1.81	0.44
1:C:429:SER:O	1:C:567:LEU:HD23	2.18	0.44
1:C:710:MET:HE1	1:C:715:ILE:HD12	2.00	0.44
1:D:651:HIS:HD2	1:D:659:ARG:CZ	2.31	0.44
1:A:272:HIS:CD2	1:A:290:PRO:HB3	2.52	0.44
1:A:278:THR:HG22	1:A:304:LEU:HD23	2.00	0.44
1:A:397:LYS:HD2	1:A:455:TYR:HB3	1.99	0.44
1:A:468:PHE:HE2	1:A:534:VAL:HG12	1.83	0.44
1:A:870:GLN:HE21	1:A:870:GLN:HB2	1.52	0.44
1:A:915:LYS:O	1:A:919:GLU:HG3	2.18	0.44
1:B:659:ARG:O	1:B:663:ILE:HG13	2.18	0.44
1:B:918:PHE:CE2	1:B:931:PHE:HA	2.52	0.44
1:C:337:GLU:HG3	1:C:374:HIS:HB3	1.98	0.44
1:D:660:VAL:HG12	1:D:695:ALA:HA	2.00	0.44
1:B:348:SER:HB3	1:B:367:VAL:HG11	2.00	0.43
1:B:496:TRP:HB2	1:B:535:LYS:HG3	1.99	0.43
1:C:186:THR:O	1:C:189:GLY:N	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:547:ILE:HG23	1:C:566:PHE:HB3	2.00	0.43
1:D:640:TRP:CH2	1:D:666:VAL:HG22	2.53	0.43
1:A:843:LEU:HB2	1:A:850:ILE:HD12	1.99	0.43
1:B:104:ALA:HB2	1:B:158:PRO:HD3	1.99	0.43
1:B:200:GLU:OE1	1:B:262:TYR:CE1	2.71	0.43
1:B:715:ILE:HD13	1:B:949:LEU:HD11	2.00	0.43
1:C:123:GLN:HB2	1:C:163:TYR:HB2	2.00	0.43
1:D:363:TRP:HZ2	8:D:1006:USK:C12	2.32	0.43
1:D:739:TRP:CZ2	1:D:755:LEU:HD22	2.54	0.43
1:A:352:ASP:O	1:A:356:SER:HB2	2.19	0.43
1:B:200:GLU:HA	1:B:201:PRO:HA	1.77	0.43
1:B:624:ASN:HB2	1:B:631:TYR:CE2	2.53	0.43
1:B:722:LEU:HA	1:B:722:LEU:HD23	1.66	0.43
1:C:820:GLU:O	1:C:824:ILE:HG13	2.18	0.43
1:D:179:PHE:CE1	1:D:195:ALA:HB1	2.53	0.43
1:D:372:LEU:HD23	1:D:372:LEU:HA	1.65	0.43
1:A:62:PHE:CD1	1:A:142:TYR:HB2	2.53	0.43
1:A:278:THR:HG21	1:A:307:LEU:HD23	2.00	0.43
1:A:446:ILE:O	1:A:449:MET:N	2.34	0.43
1:A:824:ILE:O	1:A:828:LEU:HG	2.18	0.43
1:B:456:ASN:OD1	1:B:456:ASN:N	2.52	0.43
1:B:547:ILE:HD12	1:B:548:PRO:HD2	2.00	0.43
1:A:479:ILE:O	1:A:483:LYS:HG3	2.17	0.43
1:B:371:GLU:O	1:B:374:HIS:HB2	2.18	0.43
1:C:172:LEU:HD23	1:C:172:LEU:HA	1.76	0.43
1:D:124:SER:HB2	1:D:162:TYR:CD1	2.54	0.43
1:D:738:SER:O	1:D:739:TRP:HB2	2.19	0.43
1:D:786:ILE:H	1:D:786:ILE:HG12	1.60	0.43
1:A:345:ARG:HD2	1:A:347:THR:HG22	2.01	0.43
1:A:377:PHE:CE2	1:A:395:PHE:CD1	3.06	0.43
1:A:796:SER:O	1:A:800:GLN:HG2	2.18	0.43
1:B:217:LYS:HG2	1:B:259:MET:C	2.44	0.43
1:D:915:LYS:HD3	1:D:935:LEU:CD1	2.48	0.43
1:A:215:LEU:HD12	1:A:384:GLU:HG2	2.01	0.43
1:A:718:ILE:HD11	1:A:953:ARG:HB2	2.00	0.43
1:A:907:SER:HB3	11:A:1013:BR:BR	2.74	0.43
1:C:201:PRO:HB2	1:C:202:THR:HG23	2.00	0.43
1:C:434:ARG:NH2	1:C:454:SER:OG	2.48	0.43
1:C:568:GLN:HB3	1:C:940:LYS:NZ	2.33	0.43
1:D:837:LEU:HD22	1:D:862:ILE:HD13	2.01	0.43
1:B:957:MET:O	1:B:960:THR:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:614:LEU:HD23	1:C:614:LEU:N	2.34	0.43
1:D:184:TYR:HB3	1:D:329:PRO:HG2	2.01	0.43
1:D:790:VAL:HG12	1:D:794:VAL:CG2	2.47	0.43
1:A:342:ILE:HG21	1:A:371:GLU:HB3	2.00	0.43
1:A:587:HIS:CD2	1:A:606:LYS:HG2	2.53	0.43
1:B:843:LEU:HD13	1:B:849:VAL:HG11	2.01	0.43
1:B:928:LEU:CB	1:B:930:ILE:HG22	2.42	0.43
1:C:860:HIS:HD2	1:C:900:GLY:CA	2.30	0.43
1:A:377:PHE:CE1	1:A:482:LEU:HD11	2.54	0.43
1:A:550:LEU:HD12	1:A:562:GLN:O	2.19	0.43
1:A:838:LEU:HD13	1:A:871:LEU:HD11	2.01	0.43
1:B:496:TRP:CB	1:B:535:LYS:HG3	2.49	0.43
1:C:127:ASP:OD2	1:C:129:ARG:NH1	2.52	0.43
1:C:196:VAL:HG22	1:C:197:THR:N	2.34	0.43
1:C:309:PHE:CZ	1:C:402:ILE:HG22	2.51	0.43
1:C:318:TYR:CE2	1:C:320:LEU:HB2	2.54	0.43
1:C:846:GLU:OE2	1:C:848:LYS:HB2	2.18	0.43
1:D:236:MET:SD	1:D:320:LEU:HD22	2.59	0.43
1:D:666:VAL:HG21	1:D:683:MET:CE	2.49	0.43
1:D:929:ASP:O	1:D:932:GLN:HG2	2.19	0.43
1:A:894:ILE:HD13	1:A:894:ILE:HA	1.79	0.42
1:B:136:GLU:C	1:B:137:LEU:HD12	2.44	0.42
1:B:916:LEU:O	1:B:916:LEU:HG	2.19	0.42
1:C:906:SER:O	1:C:942:ILE:HG12	2.19	0.42
1:D:457:LYS:HG3	1:D:630:TYR:CE2	2.54	0.42
1:D:552:VAL:HG12	1:D:635:TYR:CD1	2.54	0.42
1:D:829:SER:HB2	1:D:862:ILE:HG12	2.01	0.42
1:A:98:GLU:HG3	1:A:163:TYR:CE2	2.54	0.42
1:A:358:ALA:HB2	1:A:748:ARG:NE	2.33	0.42
1:A:840:LEU:HD23	1:A:840:LEU:HA	1.77	0.42
1:B:140:LEU:HD11	1:B:151:LEU:HD11	2.01	0.42
1:B:307:LEU:HD13	1:B:372:LEU:HD13	2.01	0.42
1:D:274:LEU:HA	1:D:274:LEU:HD12	1.53	0.42
1:D:412:GLN:OE1	1:D:746:TRP:HD1	2.02	0.42
1:D:422:PHE:HA	1:D:425:ILE:HD12	2.02	0.42
1:A:326:ILE:CG2	1:A:343:THR:HG22	2.49	0.42
1:A:332:ALA:N	1:A:333:PRO:HD2	2.35	0.42
1:C:486:SER:HB3	1:C:487:TYR:CD1	2.54	0.42
1:C:671:GLY:HA2	1:C:944:TRP:CD1	2.54	0.42
1:D:223:LYS:HE3	1:D:252:HIS:CE1	2.55	0.42
1:D:884:LEU:HD23	1:D:884:LEU:HA	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LEU:HD23	1:A:187:LEU:O	2.19	0.42
1:B:825:LEU:HA	1:B:825:LEU:HD12	1.77	0.42
1:C:220:PHE:CZ	1:C:261:THR:HG22	2.53	0.42
1:C:325:LEU:HD23	1:C:344:TYR:CE2	2.53	0.42
1:C:552:VAL:HB	1:C:635:TYR:HD1	1.84	0.42
1:C:892:TYR:HB2	8:C:1006:USK:C30	2.49	0.42
1:D:401:LEU:HD13	1:D:417:PHE:CB	2.49	0.42
1:D:429:SER:O	1:D:567:LEU:HD23	2.19	0.42
1:D:740:SER:HA	1:D:787:PRO:CG	2.49	0.42
1:D:915:LYS:HD3	1:D:935:LEU:HD11	2.01	0.42
1:A:375:GLN:HB2	1:A:376:TRP:CE3	2.55	0.42
1:A:449:MET:HB3	1:A:449:MET:HE3	1.79	0.42
1:A:479:ILE:HG22	1:A:483:LYS:HD2	2.00	0.42
1:B:69:LEU:HD13	1:B:211:PHE:HD1	1.84	0.42
1:B:131:MET:O	1:B:134:GLY:N	2.51	0.42
1:B:385:TRP:CG	1:B:386:TRP:H	2.38	0.42
1:B:450:PHE:O	8:B:1005:USK:O34	2.37	0.42
1:B:532:ALA:C	12:B:1107:HOH:O	2.61	0.42
1:B:674:ARG:NH1	12:B:1112:HOH:O	2.49	0.42
1:B:693:SER:N	1:B:694:PRO:HD2	2.33	0.42
1:B:799:ALA:HB1	1:B:805:TRP:HD1	1.83	0.42
1:C:731:LYS:N	1:C:732:PRO:HD2	2.35	0.42
1:D:552:VAL:HG12	1:D:635:TYR:HD1	1.84	0.42
1:D:563:GLN:O	1:D:563:GLN:HG3	2.19	0.42
1:D:650:ASN:OD1	1:D:652:THR:HG22	2.19	0.42
1:D:889:LEU:CD1	1:D:926:SER:HB3	2.50	0.42
1:D:954:THR:O	1:D:958:VAL:HG23	2.20	0.42
1:A:381:VAL:HG21	1:A:482:LEU:HA	2.01	0.42
1:B:469:LEU:HD22	1:B:473:LYS:HD2	2.00	0.42
1:B:543:LEU:HD23	1:B:543:LEU:HA	1.78	0.42
1:D:236:MET:HG3	1:D:254:GLU:O	2.19	0.42
1:A:740:SER:OG	1:A:742:LYS:HG2	2.20	0.42
1:B:116:GLU:O	1:B:168:PHE:HA	2.20	0.42
1:B:152:VAL:HG22	12:B:1103:HOH:O	2.20	0.42
1:B:563:GLN:HG3	1:B:588:ILE:HD11	2.02	0.42
1:B:718:ILE:HG21	1:B:718:ILE:HD13	1.68	0.42
1:D:380:LEU:HG	1:D:486:SER:HA	2.02	0.42
1:A:884:LEU:HA	1:A:884:LEU:HD23	1.71	0.42
1:B:82:VAL:HB	1:B:224:ILE:HD13	2.01	0.42
1:B:137:LEU:HD23	1:B:150:LEU:HB3	2.01	0.42
1:B:377:PHE:CZ	1:B:482:LEU:HD11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:GLU:H	1:B:410:GLU:HG2	1.59	0.42
1:B:885:LYS:HA	1:B:885:LYS:HD2	1.64	0.42
1:B:934:VAL:O	1:B:938:ILE:HG13	2.20	0.42
1:D:566:PHE:CD2	1:D:632:ILE:HD12	2.54	0.42
1:D:818:SER:HA	1:D:821:GLN:HB2	2.02	0.42
1:B:596:SER:OG	1:B:597:SER:N	2.53	0.42
1:C:56:ALA:HB3	1:C:60:GLU:O	2.19	0.42
1:C:257:VAL:HB	1:C:487:TYR:HE2	1.85	0.42
1:D:151:LEU:HD23	1:D:151:LEU:HA	1.80	0.42
1:D:791:LEU:HD11	1:D:795:TYR:CE2	2.55	0.42
1:A:577:TRP:CZ2	1:A:581:GLN:HG3	2.55	0.42
1:B:828:LEU:HB3	1:B:840:LEU:HD11	2.01	0.42
1:A:113:LYS:HD2	1:A:206:MET:HE2	2.02	0.41
1:A:703:LEU:HA	1:A:703:LEU:HD12	1.80	0.41
1:A:763:HIS:CE1	1:A:765:PRO:HD2	2.55	0.41
1:B:595:SER:HB2	1:B:618:THR:OG1	2.20	0.41
1:C:442:THR:HG22	1:C:444:THR:N	2.35	0.41
1:D:391:LEU:HD23	1:D:391:LEU:HA	1.87	0.41
1:A:83:HIS:ND1	1:A:225:ARG:HD2	2.34	0.41
1:A:597:SER:OG	1:A:599:VAL:HG12	2.20	0.41
1:A:700:LEU:HA	1:A:700:LEU:HD12	1.73	0.41
1:B:837:LEU:O	1:B:840:LEU:HB2	2.20	0.41
1:C:236:MET:HB3	1:C:237:PRO:HD2	2.01	0.41
1:D:796:SER:O	1:D:800:GLN:HG2	2.20	0.41
1:A:418:LEU:HD23	1:A:418:LEU:HA	1.95	0.41
1:A:667:PHE:O	1:A:670:VAL:HB	2.20	0.41
1:B:388:ASP:CG	1:B:492:ASN:HB2	2.44	0.41
1:B:907:SER:HB2	1:B:910:LYS:H	1.86	0.41
1:D:799:ALA:HB2	1:D:808:LEU:HD12	2.02	0.41
1:A:292:LYS:NZ	1:A:346:GLU:OE2	2.50	0.41
1:A:646:GLN:NE2	1:A:653:LEU:HD12	2.34	0.41
1:B:117:ILE:CD1	1:B:148:ILE:HD13	2.50	0.41
1:B:284:VAL:HA	1:B:323:LEU:O	2.21	0.41
1:C:117:ILE:HD13	1:C:148:ILE:HD13	2.02	0.41
1:C:723:LYS:HG3	1:C:761:LEU:HB3	2.01	0.41
1:C:773:LEU:HD23	1:C:773:LEU:HA	1.69	0.41
1:C:935:LEU:O	1:C:939:THR:OG1	2.36	0.41
1:D:279:SER:HB2	1:D:308:ASP:OD1	2.20	0.41
1:D:882:HIS:H	1:D:882:HIS:HD1	1.68	0.41
1:A:833:HIS:ND1	1:A:836:LYS:HE2	2.36	0.41
1:C:231:ILE:HG12	1:C:269:CYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:557:CYS:HB2	1:C:617:LYS:HG2	2.03	0.41
1:C:712:ARG:HD3	1:C:869:GLN:OE1	2.20	0.41
1:D:477:GLY:HA3	1:D:499:LEU:HD23	2.01	0.41
1:D:600:ILE:HG21	1:D:625:VAL:HG11	2.03	0.41
1:D:644:ILE:CD1	1:D:683:MET:HB2	2.51	0.41
1:A:202:THR:O	1:A:202:THR:OG1	2.32	0.41
1:B:95:GLU:O	1:B:165:ALA:HA	2.21	0.41
1:B:401:LEU:HD13	1:B:417:PHE:HB2	2.03	0.41
1:D:295:GLN:HB2	1:D:350:LEU:HG	2.02	0.41
1:D:358:ALA:HB2	1:D:748:ARG:NE	2.35	0.41
1:A:126:GLU:HB3	1:A:160:LEU:HD22	2.03	0.41
1:B:298:TYR:CE1	1:B:361:LYS:HE2	2.56	0.41
1:C:647:LEU:HD13	1:C:686:TYR:CZ	2.56	0.41
1:C:867:LYS:N	1:C:867:LYS:HD2	2.35	0.41
1:D:202:THR:O	1:D:205:ARG:HG2	2.21	0.41
1:D:239:VAL:HG23	1:D:240:LYS:H	1.85	0.41
1:D:534:VAL:HA	1:D:537:MET:HB3	2.01	0.41
1:A:663:ILE:O	1:A:666:VAL:HG12	2.21	0.41
1:B:328:ILE:HA	1:B:329:PRO:HD3	1.92	0.41
1:C:53:PHE:HB3	1:C:54:PRO:HD3	2.03	0.41
1:C:176:PHE:HD1	12:C:1112:HOH:O	2.04	0.41
1:D:384:GLU:HG2	1:D:489:ASN:HB3	2.02	0.41
1:D:565:ARG:HB3	1:D:581:GLN:HE21	1.84	0.41
1:A:168:PHE:CE2	1:A:208:PHE:HA	2.56	0.41
1:B:362:LEU:HD12	1:B:362:LEU:HA	1.82	0.41
1:B:484:LYS:HG2	1:B:485:PHE:CE1	2.56	0.41
1:B:510:SER:C	1:B:512:GLY:H	2.27	0.41
1:B:675:LEU:HD22	1:B:679:LYS:HD2	2.02	0.41
1:C:398:TYR:HD2	1:C:399:MET:HG2	1.85	0.41
1:C:697:LEU:O	1:C:701:SER:HB2	2.20	0.41
1:C:726:LEU:HD23	1:C:726:LEU:HA	1.96	0.41
1:D:64:TRP:CB	1:D:109:ILE:HD13	2.51	0.41
1:D:184:TYR:CZ	1:D:192:ARG:HB2	2.56	0.41
1:D:380:LEU:HA	1:D:380:LEU:HD12	1.72	0.41
1:D:541:TRP:HZ2	1:D:588:ILE:HA	1.85	0.41
1:D:592:TYR:C	1:D:592:TYR:CD1	2.99	0.41
1:D:710:MET:HE2	1:D:710:MET:HB3	1.77	0.41
1:D:718:ILE:HG23	1:D:956:LEU:HD12	2.03	0.41
1:D:740:SER:OG	1:D:741:ASP:N	2.54	0.41
1:D:823:LYS:O	1:D:826:TYR:HB3	2.21	0.41
1:D:859:LEU:HD21	1:D:875:PHE:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:922:GLU:HG3	1:D:923:ALA:H	1.86	0.41
1:A:278:THR:OG1	1:A:282:VAL:HG23	2.21	0.41
1:A:408:TYR:HB3	1:A:411:LEU:HG	2.02	0.41
1:A:468:PHE:CZ	1:A:604:ILE:HD11	2.55	0.41
1:A:507:ASP:N	12:A:1106:HOH:O	2.43	0.41
1:A:698:GLU:O	1:A:699:GLY:C	2.64	0.41
1:A:791:LEU:HD12	1:A:791:LEU:HA	1.82	0.41
1:B:191:THR:H	1:D:191:THR:HB	1.86	0.41
1:C:922:GLU:HG3	1:C:926:SER:O	2.21	0.41
1:D:83:HIS:CD2	1:D:83:HIS:C	2.98	0.41
1:D:895:ARG:HD2	1:D:930:ILE:HG12	2.02	0.41
1:A:550:LEU:HD21	1:A:561:LEU:HD22	2.03	0.40
1:B:184:TYR:O	1:B:191:THR:HA	2.21	0.40
1:B:830:THR:HG23	1:B:865:ARG:HH21	1.85	0.40
1:C:305:LYS:HB3	1:C:407:THR:CG2	2.51	0.40
1:C:452:GLU:HG3	8:C:1006:USK:C12	2.50	0.40
1:C:588:ILE:H	1:C:588:ILE:HG13	1.60	0.40
1:A:97:ILE:HG22	1:A:99:VAL:HG13	2.03	0.40
1:B:858:LEU:O	1:B:861:ALA:N	2.55	0.40
1:C:537:MET:O	1:C:540:THR:HB	2.21	0.40
1:C:700:LEU:HA	1:C:700:LEU:HD23	1.77	0.40
1:C:867:LYS:HD2	1:C:867:LYS:H	1.87	0.40
1:D:859:LEU:HD13	1:D:897:ILE:HG23	2.03	0.40
1:C:64:TRP:CZ3	1:C:70:PRO:HG3	2.56	0.40
1:C:351:PHE:CZ	1:C:361:LYS:HD3	2.56	0.40
1:D:152:VAL:HG21	1:D:156:LEU:HD12	2.02	0.40
1:D:895:ARG:HG3	1:D:930:ILE:HG12	2.03	0.40
1:A:710:MET:O	1:A:713:ARG:O	2.39	0.40
1:C:620:TRP:HB3	1:C:642:GLN:CG	2.51	0.40
1:D:561:LEU:HD23	1:D:605:LEU:HD22	2.04	0.40
1:D:922:GLU:C	1:D:924:GLN:N	2.80	0.40
1:A:755:LEU:HD23	1:A:755:LEU:HA	1.79	0.40
1:B:89:LEU:HD13	1:B:181:LYS:HE3	2.03	0.40
1:B:465:LEU:HD22	1:B:538:MET:HG3	2.02	0.40
1:C:110:LEU:HD11	1:C:150:LEU:HD11	2.03	0.40
1:C:810:GLU:O	1:C:814:LEU:HG	2.21	0.40
1:D:314:PHE:O	1:D:479:ILE:HG23	2.22	0.40
1:D:318:TYR:CE2	1:D:320:LEU:HB2	2.56	0.40
1:D:442:THR:OG1	1:D:445:GLN:HG3	2.21	0.40
1:D:829:SER:O	1:D:837:LEU:HD21	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	915/966 (95%)	830 (91%)	77 (8%)	8 (1%)	14	44
1	B	906/966 (94%)	845 (93%)	53 (6%)	8 (1%)	14	44
1	C	879/966 (91%)	821 (93%)	50 (6%)	8 (1%)	14	44
1	D	883/966 (91%)	831 (94%)	49 (6%)	3 (0%)	36	67
All	All	3583/3864 (93%)	3327 (93%)	229 (6%)	27 (1%)	16	47

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	615	PRO
1	B	744	SER
1	D	132	LYS
1	B	216	PHE
1	B	616	GLU
1	B	687	LEU
1	C	56	ALA
1	C	688	GLN
1	A	818	SER
1	B	294	ASN
1	C	615	PRO
1	C	684	THR
1	A	58	ASN
1	B	504	LEU
1	C	53	PHE
1	C	201	PRO
1	C	294	ASN
1	A	120	ALA
1	A	335	ALA
1	A	508	PHE
1	B	53	PHE
1	D	615	PRO

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Mol	Chain	Res	Type
1	A	329	PRO
1	C	925	GLY
1	A	402	ILE
1	A	694	PRO
1	D	201	PRO

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	812/869 (93%)	751 (92%)	61 (8%)	12	39
1	B	801/869 (92%)	743 (93%)	58 (7%)	13	40
1	C	778/869 (90%)	713 (92%)	65 (8%)	10	35
1	D	758/869 (87%)	692 (91%)	66 (9%)	9	34
All	All	3149/3476 (91%)	2899 (92%)	250 (8%)	11	37

All (250) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	VAL
1	A	58	ASN
1	A	65	GLN
1	A	86	LEU
1	A	87	THR
1	A	94	SER
1	A	102	SER
1	A	137	LEU
1	A	138	LYS
1	A	152	VAL
1	A	177	GLU
1	A	194	LEU
1	A	202	THR
1	A	234	SER
1	A	241	THR
1	A	256	THR

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Mol	Chain	Res	Type
1	A	260	SER
1	A	282	VAL
1	A	289	SER
1	A	321	SER
1	A	325	LEU
1	A	326	ILE
1	A	339	TRP
1	A	345	ARG
1	A	354	LYS
1	A	356	SER
1	A	372	LEU
1	A	383	MET
1	A	428	ASP
1	A	452	GLU
1	A	454	SER
1	A	476	LYS
1	A	498	SER
1	A	523	ASN
1	A	524	MET
1	A	534	VAL
1	A	545	LYS
1	A	551	VAL
1	A	563	GLN
1	A	604	ILE
1	A	625	VAL
1	A	651	HIS
1	A	652	THR
1	A	678	ASP
1	A	686	TYR
1	A	691	THR
1	A	694	PRO
1	A	696	LEU
1	A	697	LEU
1	A	703	LEU
1	A	716	SER
1	A	738	SER
1	A	751	ARG
1	A	762	ASN
1	A	786	ILE
1	A	830	THR
1	A	832	LYS
1	A	841	ILE

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Mol	Chain	Res	Type
1	A	859	LEU
1	A	870	GLN
1	A	907	SER
1	B	65	GLN
1	B	86	LEU
1	B	110	LEU
1	B	121	THR
1	B	131	MET
1	B	221	SER
1	B	222	ILE
1	B	228	SER
1	B	233	LEU
1	B	243	GLU
1	B	275	SER
1	B	289	SER
1	B	291	ASP
1	B	320	LEU
1	B	322	LYS
1	B	343	THR
1	B	347	THR
1	B	350	LEU
1	B	357	SER
1	B	365	THR
1	B	372	LEU
1	B	383	MET
1	B	410	GLU
1	B	428	ASP
1	B	432	SER
1	B	444	THR
1	B	497	SER
1	B	514	CYS
1	B	525	LEU
1	B	547	ILE
1	B	551	VAL
1	B	553	LYS
1	B	568	GLN
1	B	572	GLN
1	B	574	ASP
1	B	588	ILE
1	B	595	SER
1	B	609	THR
1	B	617	LYS

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Mol	Chain	Res	Type
1	B	621	VAL
1	B	674	ARG
1	B	692	SER
1	B	693	SER
1	B	709	MET
1	B	716	SER
1	B	718	ILE
1	B	719	SER
1	B	733	VAL
1	B	738	SER
1	B	773	LEU
1	B	784	LEU
1	B	838	LEU
1	B	842	GLU
1	B	862	ILE
1	B	884	LEU
1	B	907	SER
1	B	957	MET
1	B	960	THR
1	C	67	LEU
1	C	71	SER
1	C	92	VAL
1	C	97	ILE
1	C	109	ILE
1	C	110	LEU
1	C	124	SER
1	C	131	MET
1	C	181	LYS
1	C	205	ARG
1	C	224	ILE
1	C	226	ARG
1	C	228	SER
1	C	241	THR
1	C	266	TYR
1	C	275	SER
1	C	279	SER
1	C	283	LYS
1	C	289	SER
1	C	297	HIS
1	C	321	SER
1	C	328	ILE
1	C	347	THR

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Mol	Chain	Res	Type
1	C	362	LEU
1	C	382	THR
1	C	383	MET
1	C	399	MET
1	C	404	VAL
1	C	420	VAL
1	C	454	SER
1	C	466	LYS
1	C	480	GLN
1	C	498	SER
1	C	545	LYS
1	C	547	ILE
1	C	551	VAL
1	C	557	CYS
1	C	573	GLU
1	C	594	THR
1	C	604	ILE
1	C	612	LEU
1	C	613	ASP
1	C	617	LYS
1	C	621	VAL
1	C	644	ILE
1	C	652	THR
1	C	658	ASP
1	C	674	ARG
1	C	710	MET
1	C	713	ARG
1	C	716	SER
1	C	729	TYR
1	C	733	VAL
1	C	757	LEU
1	C	773	LEU
1	C	818	SER
1	C	830	THR
1	C	846	GLU
1	C	852	THR
1	C	907	SER
1	C	914	VAL
1	C	916	LEU
1	C	919	GLU
1	C	930	ILE
1	C	939	THR

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Mol	Chain	Res	Type
1	D	55	VAL
1	D	66	GLU
1	D	71	SER
1	D	82	VAL
1	D	87	THR
1	D	108	ILE
1	D	109	ILE
1	D	110	LEU
1	D	112	SER
1	D	121	THR
1	D	133	PRO
1	D	160	LEU
1	D	194	LEU
1	D	241	THR
1	D	255	THR
1	D	257	VAL
1	D	285	SER
1	D	301	GLN
1	D	321	SER
1	D	325	LEU
1	D	343	THR
1	D	357	SER
1	D	382	THR
1	D	383	MET
1	D	429	SER
1	D	432	SER
1	D	442	THR
1	D	444	THR
1	D	461	ILE
1	D	539	THR
1	D	544	GLN
1	D	547	ILE
1	D	552	VAL
1	D	557	CYS
1	D	559	LEU
1	D	562	GLN
1	D	578[A]	ARG
1	D	578[B]	ARG
1	D	592	TYR
1	D	599	VAL
1	D	614	LEU
1	D	616	GLU

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Mol	Chain	Res	Type
1	D	628	ASN
1	D	645	THR
1	D	669	LEU
1	D	676	THR
1	D	684	THR
1	D	696	LEU
1	D	700	LEU
1	D	715	ILE
1	D	717	ASP
1	D	759	CYS
1	D	760	ASP
1	D	775	SER
1	D	786	ILE
1	D	788	THR
1	D	802	THR
1	D	813	GLU
1	D	814	LEU
1	D	823	LYS
1	D	852	THR
1	D	862	ILE
1	D	884	LEU
1	D	899	SER
1	D	916	LEU
1	D	922	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	77	HIS
1	A	123	GLN
1	A	252	HIS
1	A	338	ASN
1	A	375	GLN
1	A	531	ASN
1	A	544	GLN
1	A	587	HIS
1	A	634	HIS
1	A	664	HIS
1	A	800	GLN
1	A	834	GLN
1	A	904	HIS

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Mol	Chain	Res	Type
1	B	203	GLN
1	B	230	HIS
1	B	297	HIS
1	B	375	GLN
1	B	531	ASN
1	B	544	GLN
1	B	554	GLN
1	B	562	GLN
1	B	563	GLN
1	B	568	GLN
1	B	572	GLN
1	B	737	GLN
1	B	763	HIS
1	B	800	GLN
1	B	882	HIS
1	C	123	GLN
1	C	203	GLN
1	C	297	HIS
1	C	544	GLN
1	C	563	GLN
1	C	572	GLN
1	C	581	GLN
1	C	648	ASN
1	C	728	GLN
1	C	763	HIS
1	C	860	HIS
1	C	869	GLN
1	C	959	ASN
1	D	147	GLN
1	D	230	HIS
1	D	272	HIS
1	D	489	ASN
1	D	563	GLN
1	D	646	GLN
1	D	721	ASN
1	D	728	GLN
1	D	811	GLN
1	D	869	GLN
1	D	879	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 ⓘ

41 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	2,1	14,14,15	0.59	0	17,19,21	0.73	0
2	NAG	E	2	2	14,14,15	0.49	0	17,19,21	0.52	0
2	BMA	E	3	2	11,11,12	1.93	5 (45%)	15,15,17	0.83	0
2	MAN	E	4	2	11,11,12	1.35	2 (18%)	15,15,17	1.52	1 (6%)
3	NAG	F	1	1,3	14,14,15	0.54	0	17,19,21	0.65	0
3	NAG	F	2	3	14,14,15	0.71	1 (7%)	17,19,21	0.79	0
3	NAG	G	1	1,3	14,14,15	0.90	1 (7%)	17,19,21	0.50	0
3	NAG	G	2	3	14,14,15	0.28	0	17,19,21	0.59	0
4	NAG	H	1	1,4	14,14,15	0.79	1 (7%)	17,19,21	0.48	0
4	NAG	H	2	4	14,14,15	0.39	0	17,19,21	0.63	0
4	BMA	H	3	4	11,11,12	1.18	1 (9%)	15,15,17	0.87	1 (6%)
4	NAG	I	1	1,4	14,14,15	0.89	2 (14%)	17,19,21	0.63	0
4	NAG	I	2	4	14,14,15	0.32	0	17,19,21	0.77	1 (5%)
4	BMA	I	3	4	11,11,12	1.04	1 (9%)	15,15,17	0.79	1 (6%)
3	NAG	J	1	1,3	14,14,15	0.59	1 (7%)	17,19,21	0.67	0
3	NAG	J	2	3	14,14,15	0.53	0	17,19,21	0.55	0
3	NAG	K	1	1,3	14,14,15	0.73	0	17,19,21	1.27	1 (5%)
3	NAG	K	2	3	14,14,15	0.58	0	17,19,21	0.61	0
3	NAG	L	1	1,3	14,14,15	0.24	0	17,19,21	0.65	0
3	NAG	L	2	3	14,14,15	0.78	1 (7%)	17,19,21	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	M	1	1,3	14,14,15	0.81	1 (7%)	17,19,21	1.16	1 (5%)
3	NAG	M	2	3	14,14,15	0.59	1 (7%)	17,19,21	0.64	0
5	NAG	N	1	5,1	14,14,15	0.37	0	17,19,21	0.56	0
5	NAG	N	2	5	14,14,15	0.80	1 (7%)	17,19,21	0.54	0
5	BMA	N	3	5	11,11,12	1.13	1 (9%)	15,15,17	0.93	1 (6%)
5	MAN	N	4	5	11,11,12	1.05	1 (9%)	15,15,17	1.27	1 (6%)
5	MAN	N	5	5	11,11,12	1.74	5 (45%)	15,15,17	0.81	0
4	NAG	O	1	1,4	14,14,15	0.50	0	17,19,21	0.46	0
4	NAG	O	2	4	14,14,15	0.37	0	17,19,21	0.57	0
4	BMA	O	3	4	11,11,12	2.17	3 (27%)	15,15,17	1.08	1 (6%)
3	NAG	P	1	1,3	14,14,15	0.33	0	17,19,21	0.69	0
3	NAG	P	2	3	14,14,15	0.49	0	17,19,21	1.25	2 (11%)
2	NAG	Q	1	2,1	14,14,15	0.53	0	17,19,21	0.43	0
2	NAG	Q	2	2	14,14,15	0.53	0	17,19,21	0.85	1 (5%)
2	BMA	Q	3	2	11,11,12	1.05	2 (18%)	15,15,17	1.26	2 (13%)
2	MAN	Q	4	2	11,11,12	1.51	2 (18%)	15,15,17	1.06	1 (6%)
4	NAG	R	1	1,4	14,14,15	0.50	0	17,19,21	0.56	0
4	NAG	R	2	4	14,14,15	0.54	0	17,19,21	0.63	0
4	BMA	R	3	4	11,11,12	1.62	3 (27%)	15,15,17	2.03	2 (13%)
3	NAG	S	1	1,3	14,14,15	0.25	0	17,19,21	0.85	1 (5%)
3	NAG	S	2	3	14,14,15	0.90	1 (7%)	17,19,21	0.66	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
2	MAN	E	4	2	-	2/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	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	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	4/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	H	3	4	-	0/2/19/22	0/1/1/1
4	NAG	I	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	BMA	I	3	4	-	0/2/19/22	0/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	1/6/23/26	0/1/1/1
3	NAG	M	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
5	NAG	N	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	N	2	5	-	2/6/23/26	0/1/1/1
5	BMA	N	3	5	-	2/2/19/22	0/1/1/1
5	MAN	N	4	5	-	2/2/19/22	0/1/1/1
5	MAN	N	5	5	-	0/2/19/22	0/1/1/1
4	NAG	O	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
4	BMA	O	3	4	-	2/2/19/22	0/1/1/1
3	NAG	P	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	2/6/23/26	0/1/1/1
2	NAG	Q	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	2/6/23/26	0/1/1/1
2	BMA	Q	3	2	-	2/2/19/22	0/1/1/1
2	MAN	Q	4	2	-	0/2/19/22	0/1/1/1
4	NAG	R	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	R	2	4	-	0/6/23/26	0/1/1/1
4	BMA	R	3	4	-	1/2/19/22	0/1/1/1
3	NAG	S	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	3	BMA	C2-C3	4.93	1.60	1.52
2	Q	4	MAN	C2-C3	3.77	1.58	1.52
2	E	3	BMA	C4-C5	3.50	1.60	1.53
4	O	3	BMA	C4-C5	3.22	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	3	BMA	C1-C2	3.16	1.59	1.52
4	O	3	BMA	O5-C5	3.13	1.49	1.43
3	G	1	NAG	O5-C1	-3.00	1.38	1.43
5	N	2	NAG	O5-C1	-2.95	1.38	1.43
3	S	2	NAG	O5-C1	2.94	1.48	1.43
4	R	3	BMA	O5-C5	2.89	1.49	1.43
2	E	3	BMA	C2-C3	2.88	1.56	1.52
4	H	1	NAG	O5-C1	-2.72	1.39	1.43
2	E	3	BMA	O3-C3	2.71	1.49	1.43
5	N	5	MAN	O5-C1	-2.68	1.39	1.43
3	L	2	NAG	C1-C2	2.66	1.56	1.52
2	E	4	MAN	C1-C2	2.65	1.58	1.52
5	N	5	MAN	C2-C3	2.57	1.56	1.52
5	N	5	MAN	C4-C5	2.56	1.58	1.53
4	R	3	BMA	O5-C1	2.45	1.47	1.43
2	E	3	BMA	C4-C3	2.43	1.58	1.52
5	N	5	MAN	O5-C5	2.42	1.48	1.43
3	F	2	NAG	C1-C2	2.38	1.55	1.52
5	N	4	MAN	O5-C5	2.33	1.48	1.43
2	E	4	MAN	O5-C5	2.32	1.47	1.43
3	M	1	NAG	C1-C2	2.30	1.55	1.52
4	I	1	NAG	O5-C1	-2.28	1.39	1.43
2	Q	3	BMA	C4-C5	2.16	1.57	1.53
4	I	3	BMA	C4-C3	2.15	1.57	1.52
3	J	1	NAG	C1-C2	2.10	1.55	1.52
4	H	3	BMA	C4-C3	2.08	1.57	1.52
5	N	5	MAN	C4-C3	2.08	1.57	1.52
4	I	1	NAG	C1-C2	2.07	1.55	1.52
2	Q	3	BMA	C2-C3	2.07	1.55	1.52
5	N	3	BMA	C4-C3	2.04	1.57	1.52
3	M	2	NAG	C1-C2	2.03	1.55	1.52
2	Q	4	MAN	C1-C2	2.03	1.57	1.52
2	E	3	BMA	O5-C5	2.02	1.47	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	3	BMA	C1-O5-C5	6.76	121.25	112.19
2	E	4	MAN	C1-O5-C5	5.13	119.06	112.19
3	M	1	NAG	C1-O5-C5	4.08	117.65	112.19
3	P	2	NAG	C2-N2-C7	4.04	128.31	122.90
5	N	4	MAN	C1-O5-C5	3.51	116.89	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	1	NAG	C1-C2-N2	3.20	115.48	110.43
2	Q	3	BMA	C2-C3-C4	3.01	116.15	110.86
4	O	3	BMA	O3-C3-C2	2.75	115.67	110.05
3	S	1	NAG	C1-O5-C5	2.71	115.82	112.19
3	P	2	NAG	C1-C2-N2	2.71	114.70	110.43
2	Q	2	NAG	C1-O5-C5	2.40	115.40	112.19
4	I	3	BMA	C1-O5-C5	2.35	115.33	112.19
5	N	3	BMA	O2-C2-C3	-2.26	105.47	110.15
4	H	3	BMA	O2-C2-C3	-2.19	105.61	110.15
4	R	3	BMA	O5-C1-C2	2.17	115.97	110.79
2	Q	3	BMA	C3-C4-C5	2.17	114.16	110.23
4	I	2	NAG	C1-O5-C5	2.15	115.07	112.19
2	Q	4	MAN	O3-C3-C2	2.13	114.40	110.05

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	P	2	NAG	C1-C2-N2-C7
3	S	2	NAG	O5-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
5	N	2	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6
3	S	2	NAG	C4-C5-C6-O6
5	N	1	NAG	O5-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
4	O	3	BMA	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	Q	2	NAG	C4-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
5	N	2	NAG	C4-C5-C6-O6
4	O	3	BMA	C4-C5-C6-O6
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
3	M	2	NAG	C8-C7-N2-C2
3	M	2	NAG	O7-C7-N2-C2
2	E	4	MAN	O5-C5-C6-O6
2	Q	1	NAG	O5-C5-C6-O6
5	N	1	NAG	C4-C5-C6-O6
2	Q	1	NAG	C4-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	J	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	S	1	NAG	C4-C5-C6-O6
2	Q	3	BMA	C4-C5-C6-O6
5	N	4	MAN	O5-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
4	R	3	BMA	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
2	Q	3	BMA	O5-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6
2	E	4	MAN	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
5	N	3	BMA	C4-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6
5	N	3	BMA	O5-C5-C6-O6
3	L	2	NAG	C3-C2-N2-C7
3	K	1	NAG	C4-C5-C6-O6
5	N	4	MAN	C4-C5-C6-O6
3	F	2	NAG	C1-C2-N2-C7
3	K	1	NAG	C1-C2-N2-C7
4	O	1	NAG	C1-C2-N2-C7
4	H	2	NAG	C4-C5-C6-O6

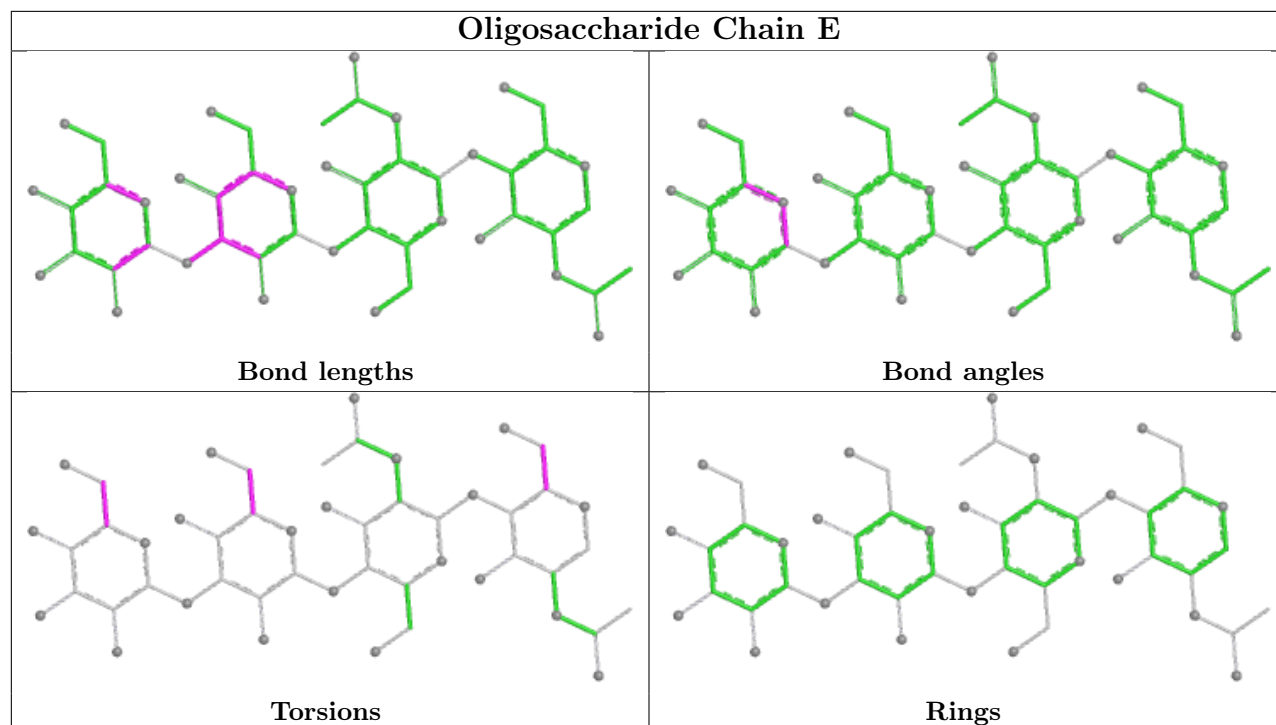
There are no ring outliers.

4 monomers are involved in 4 short contacts:

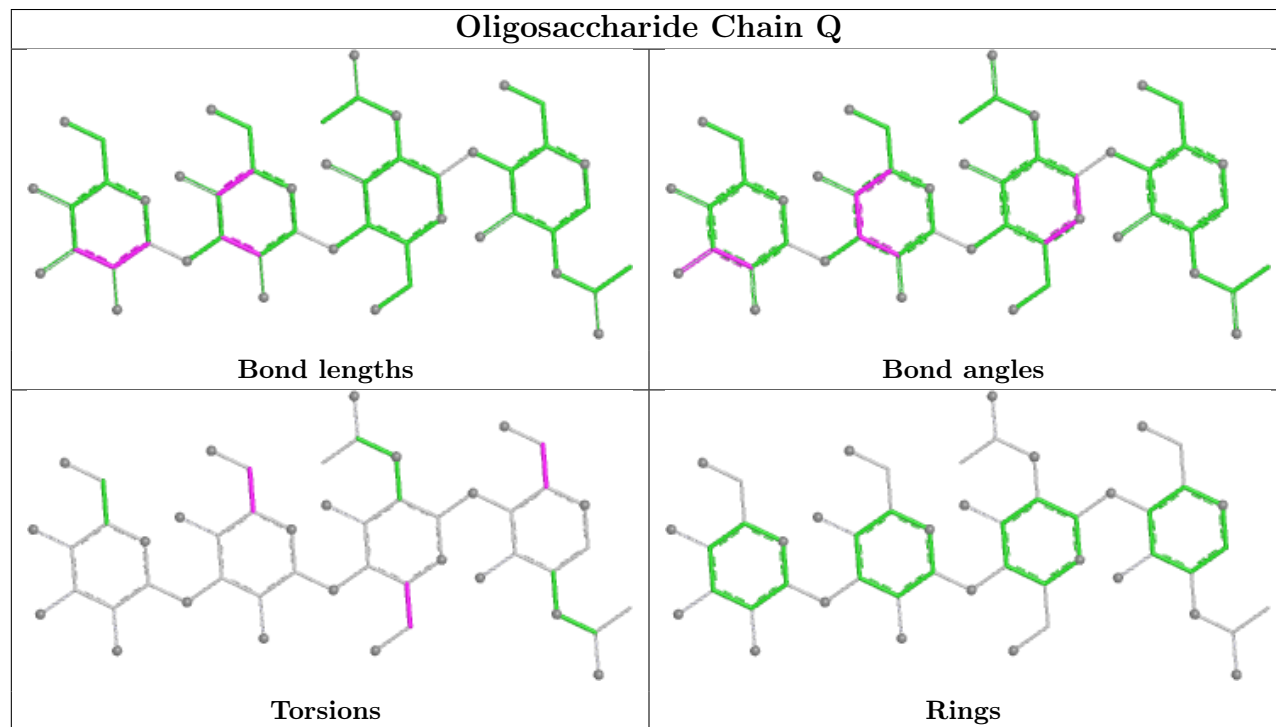
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	R	1	NAG	1	0
3	L	2	NAG	1	0
3	K	1	NAG	1	0
4	H	1	NAG	1	0

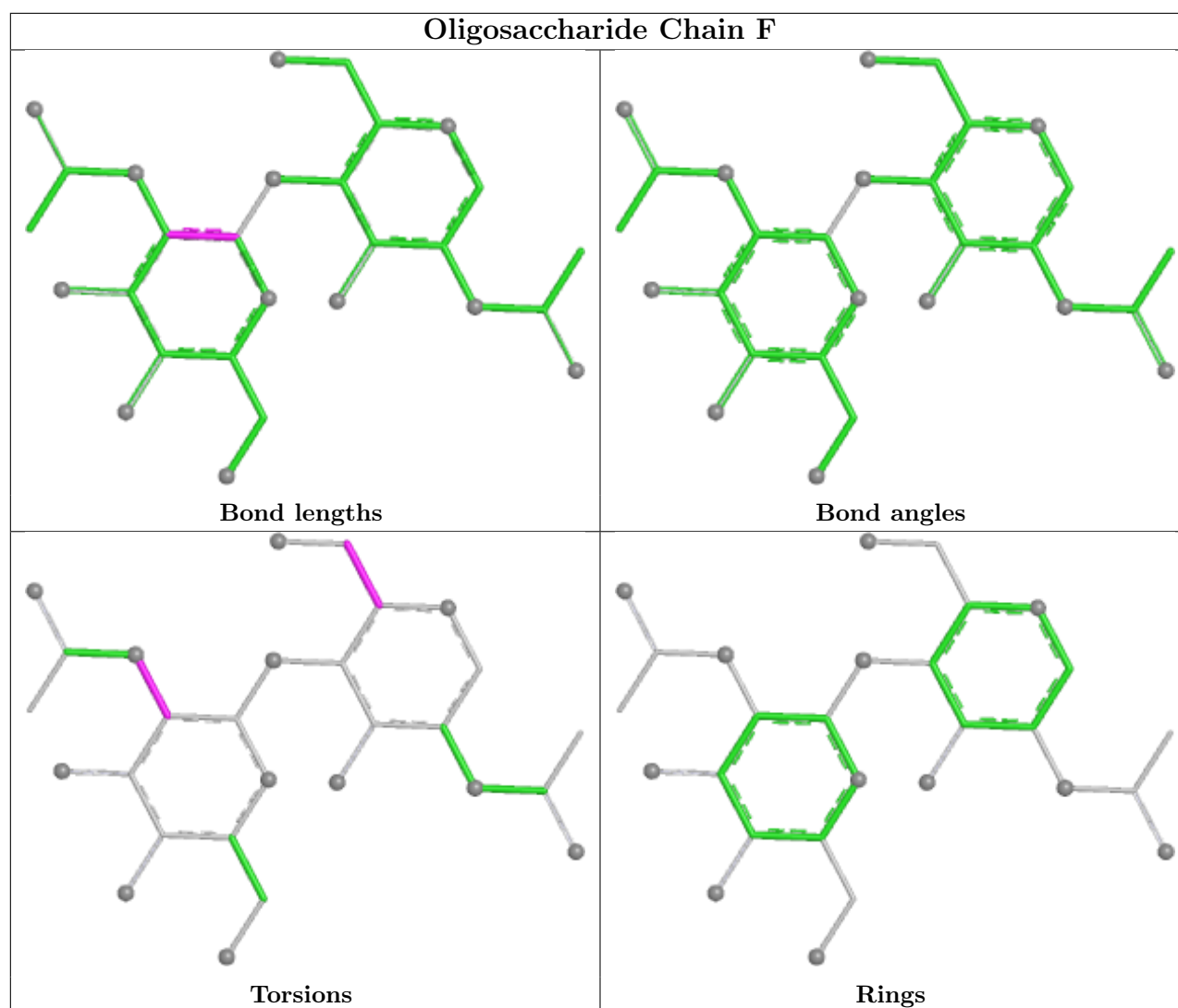
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

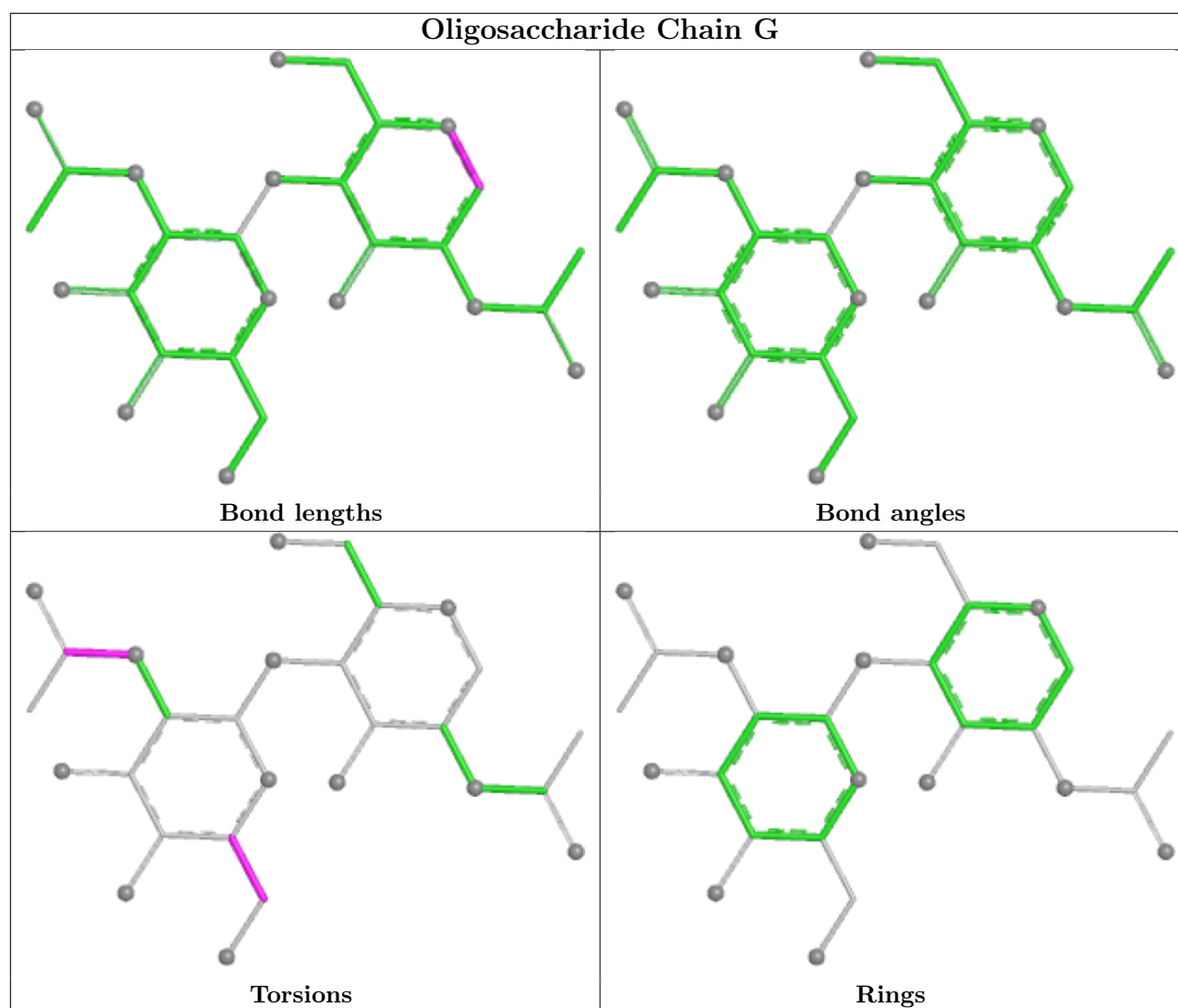
Oligosaccharide Chain E

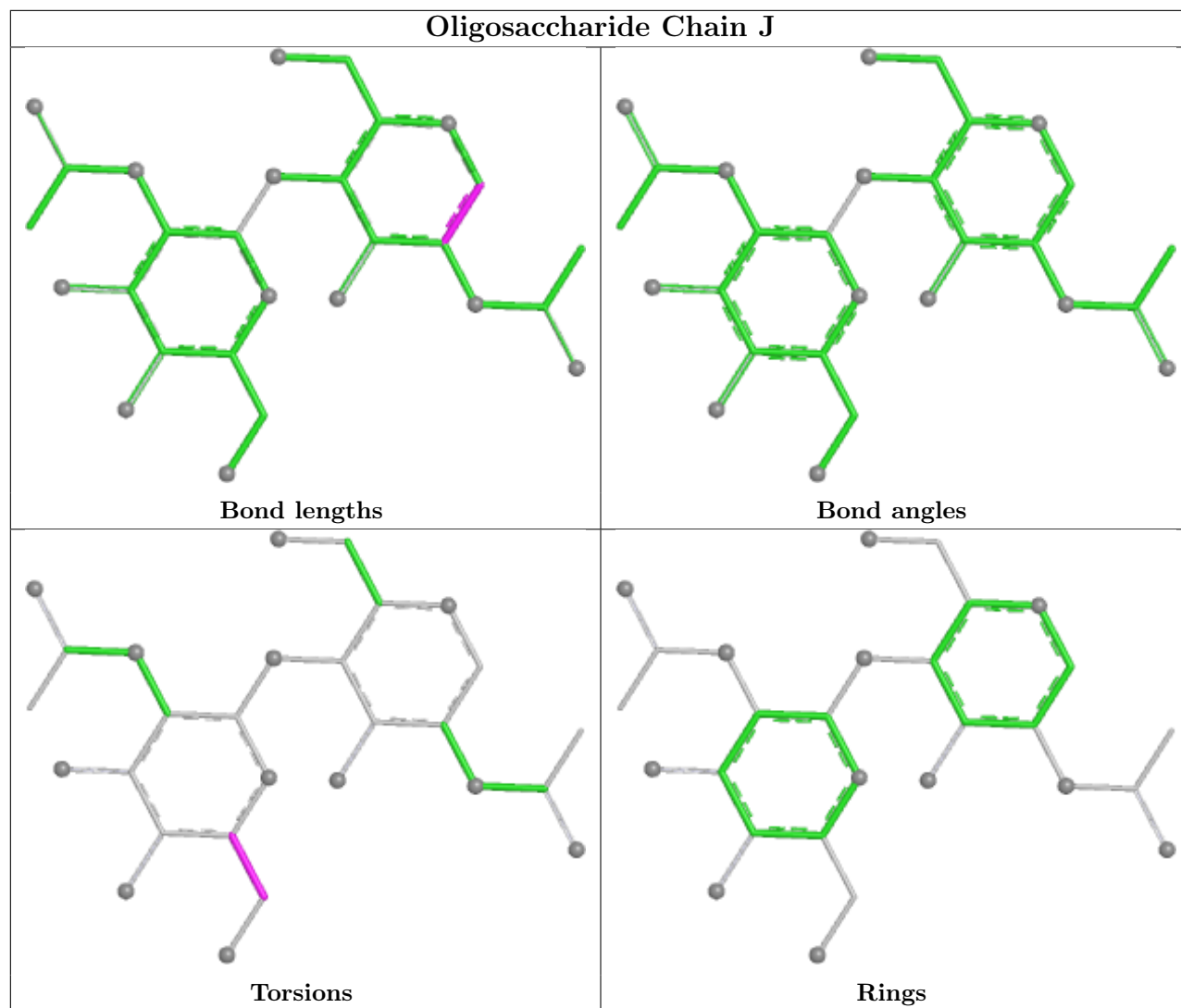


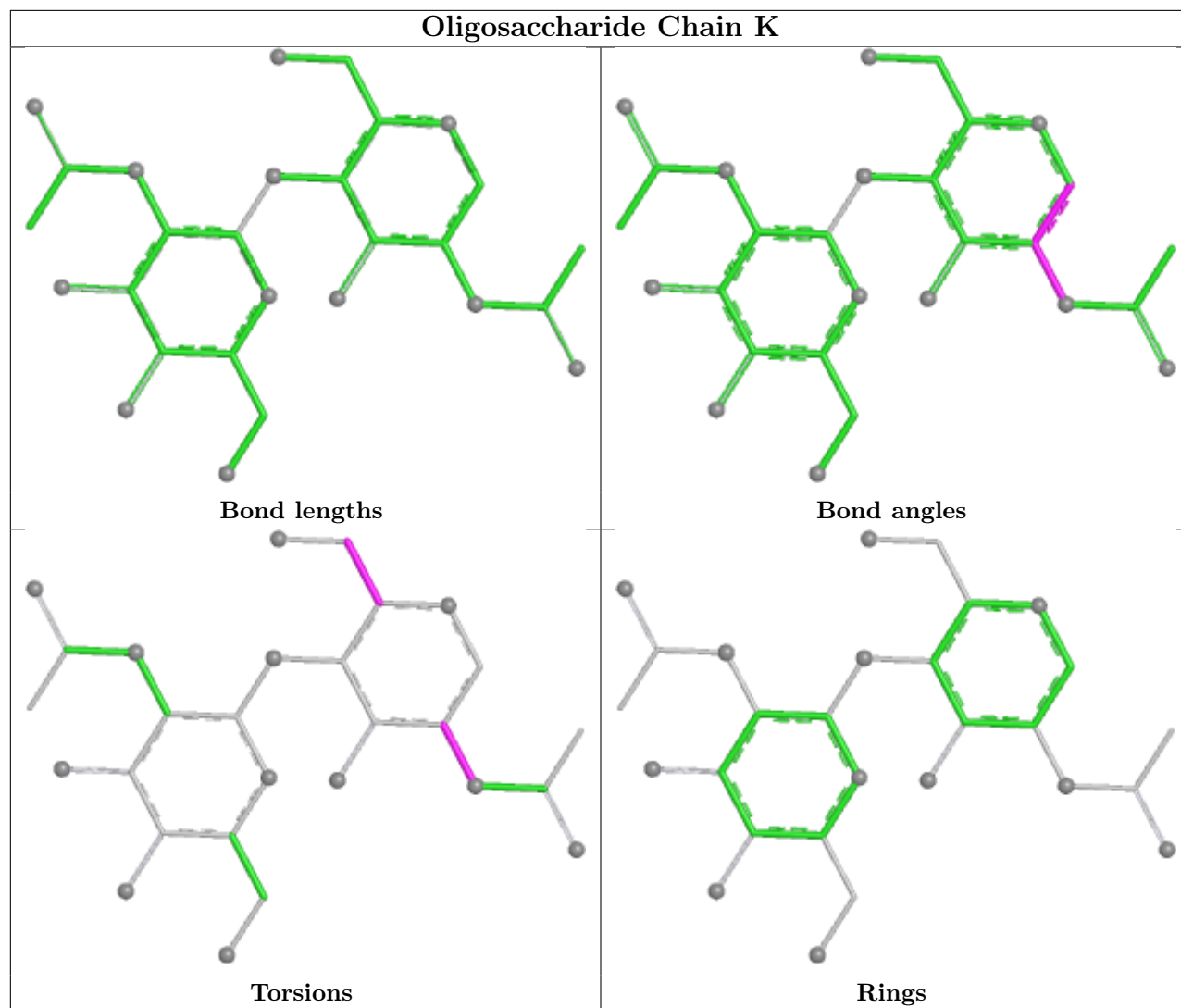
Oligosaccharide Chain Q

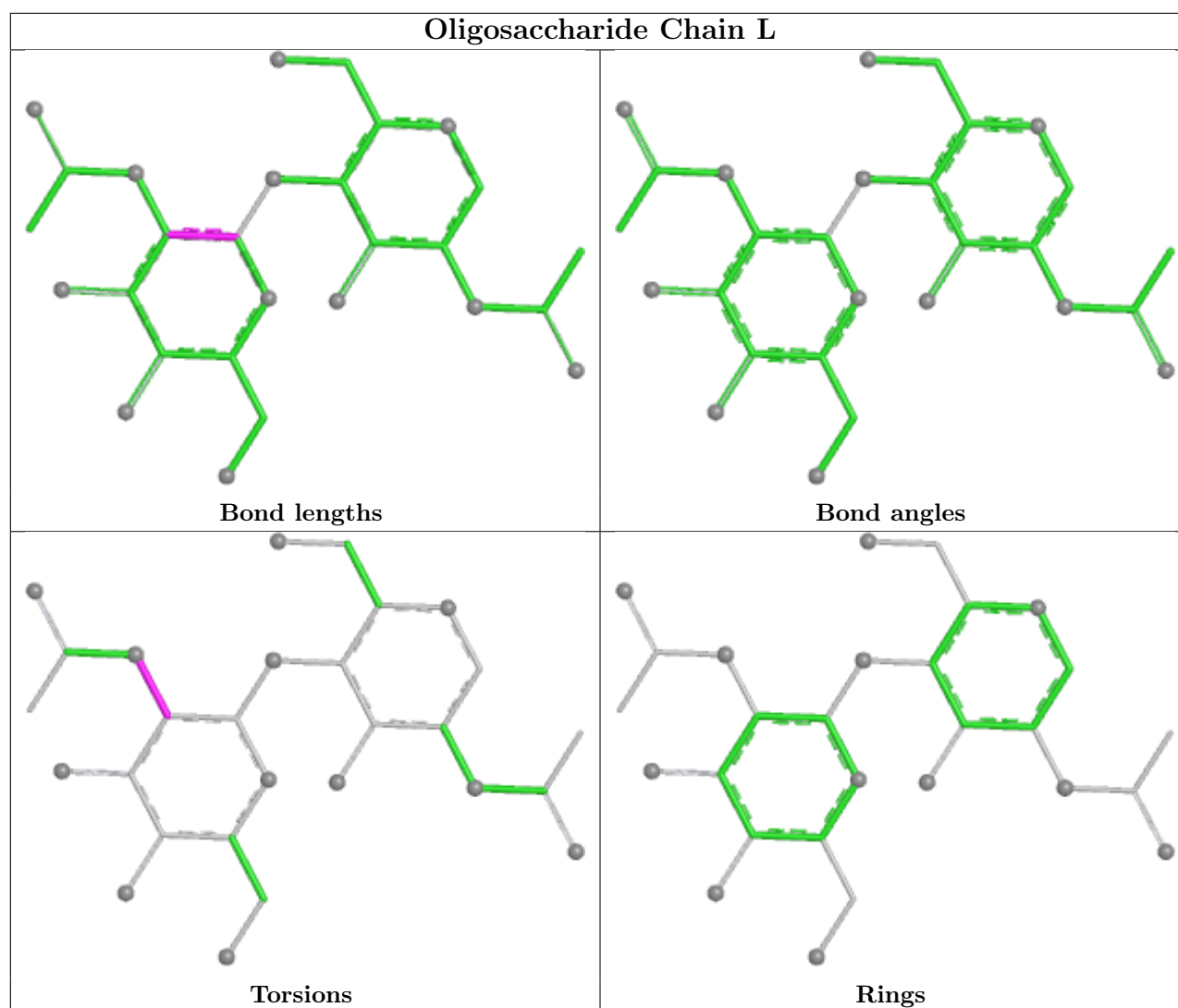


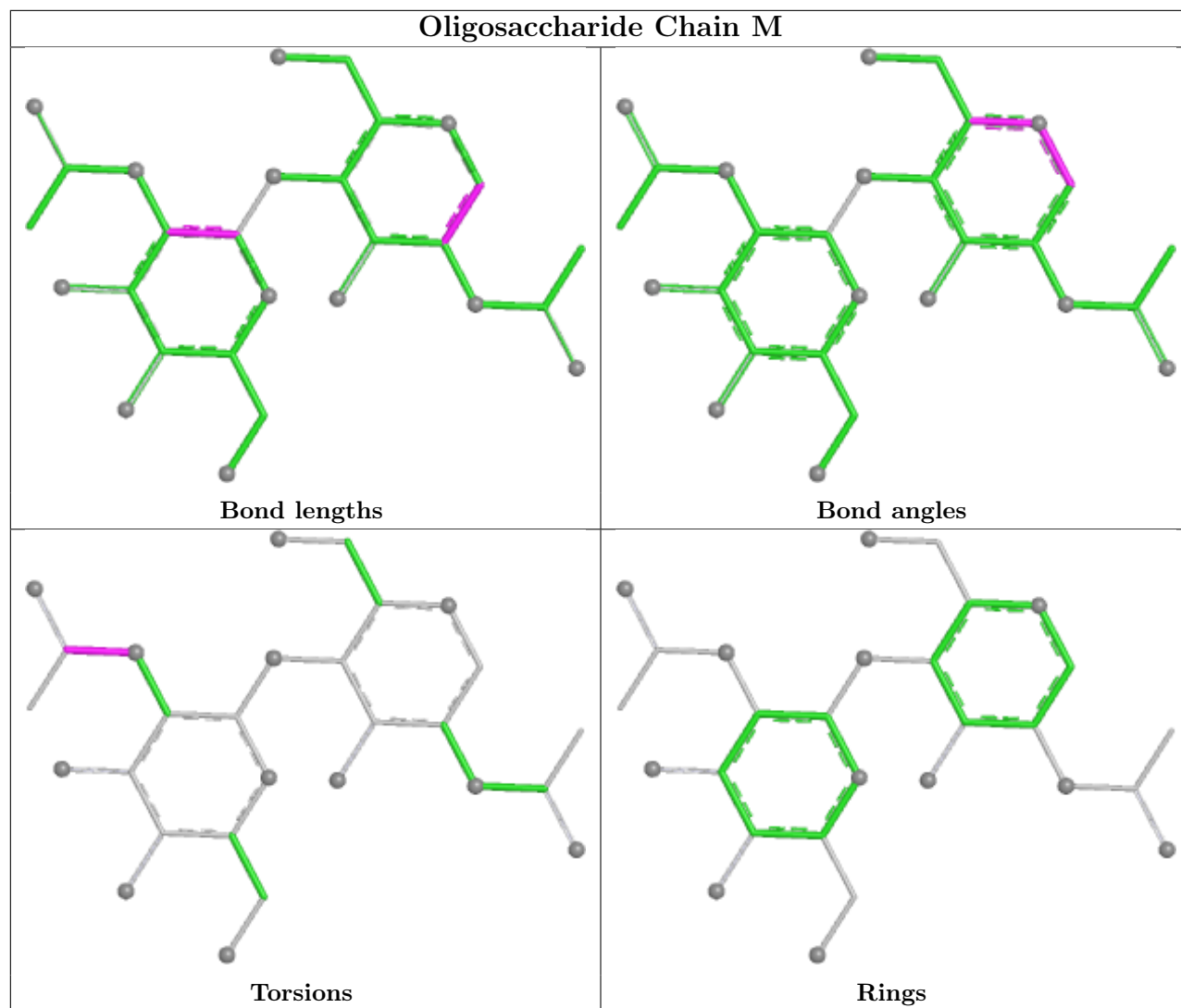


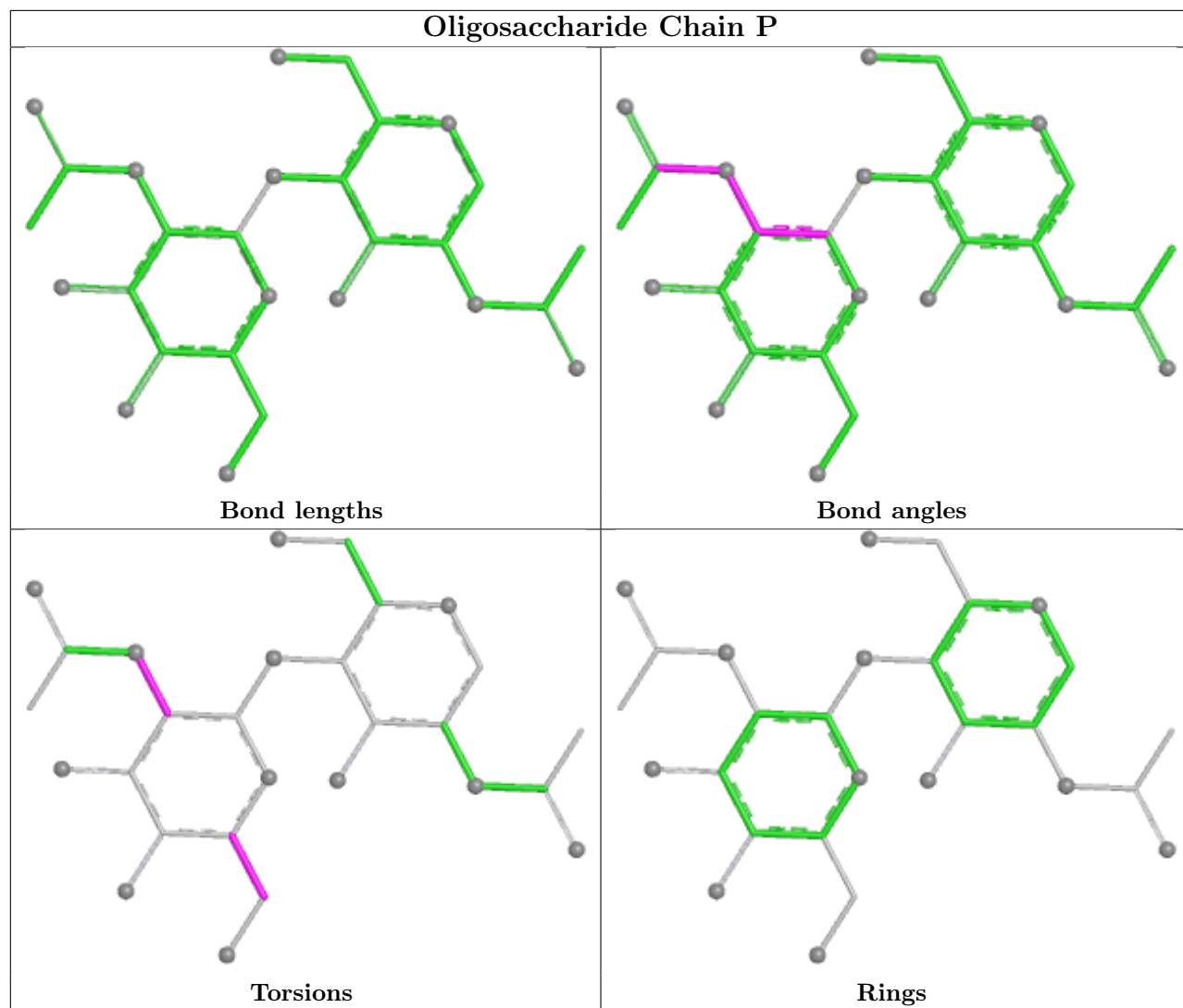


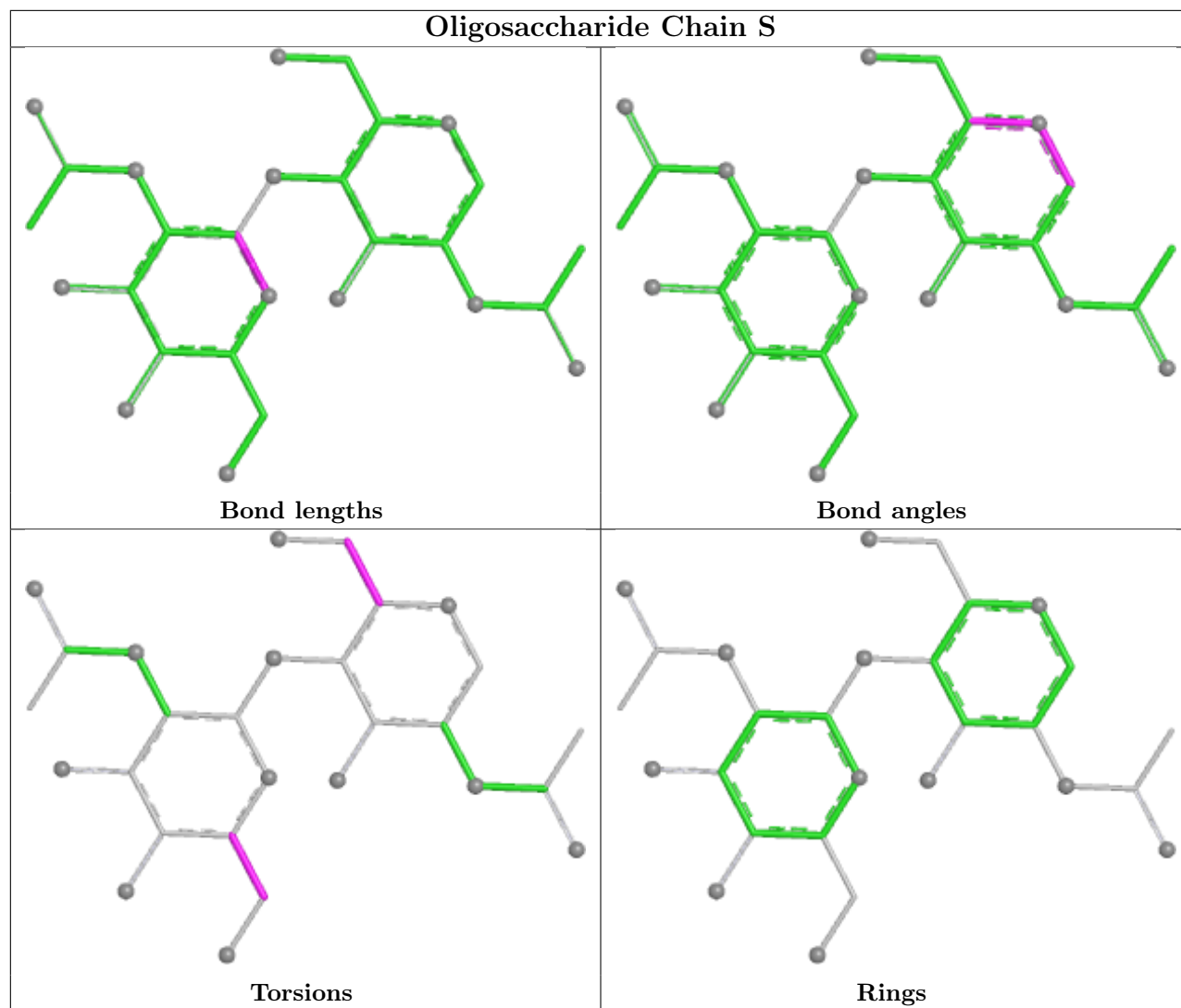


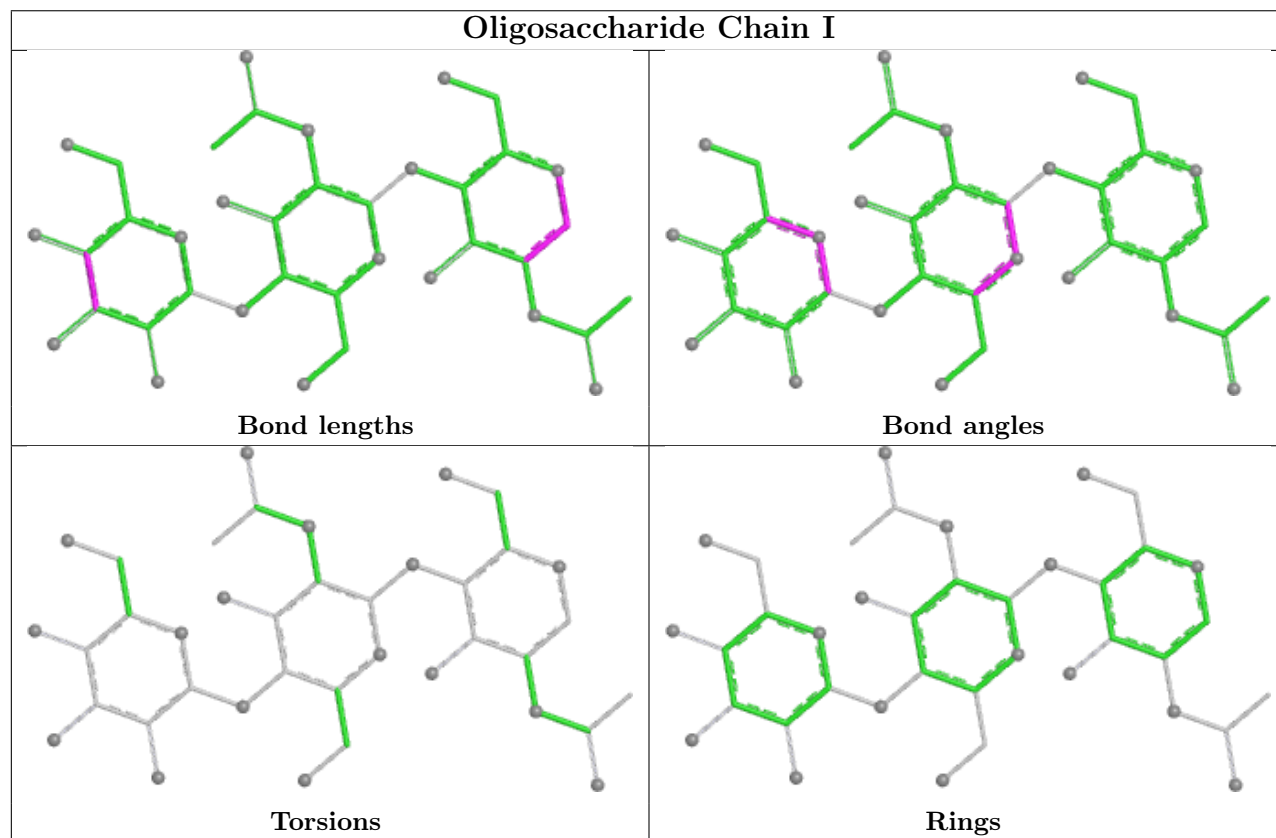
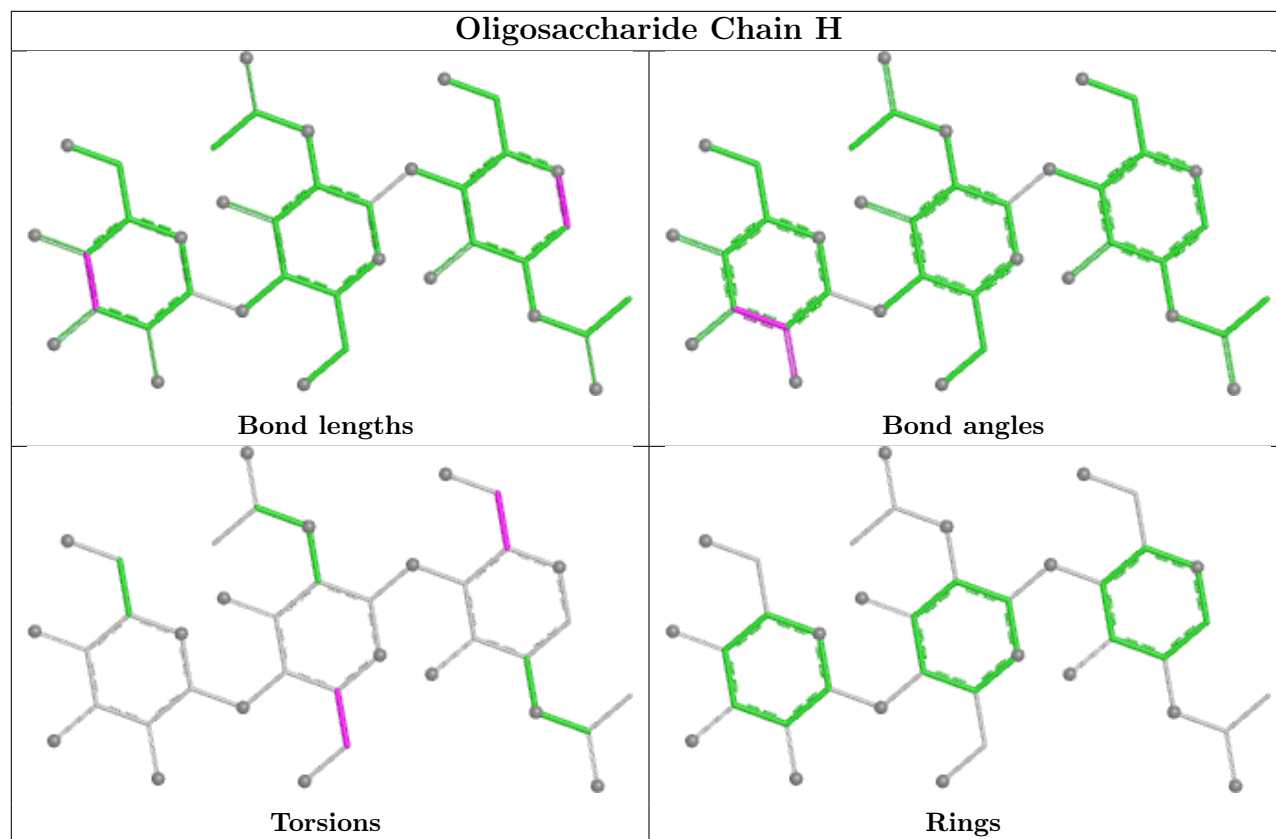


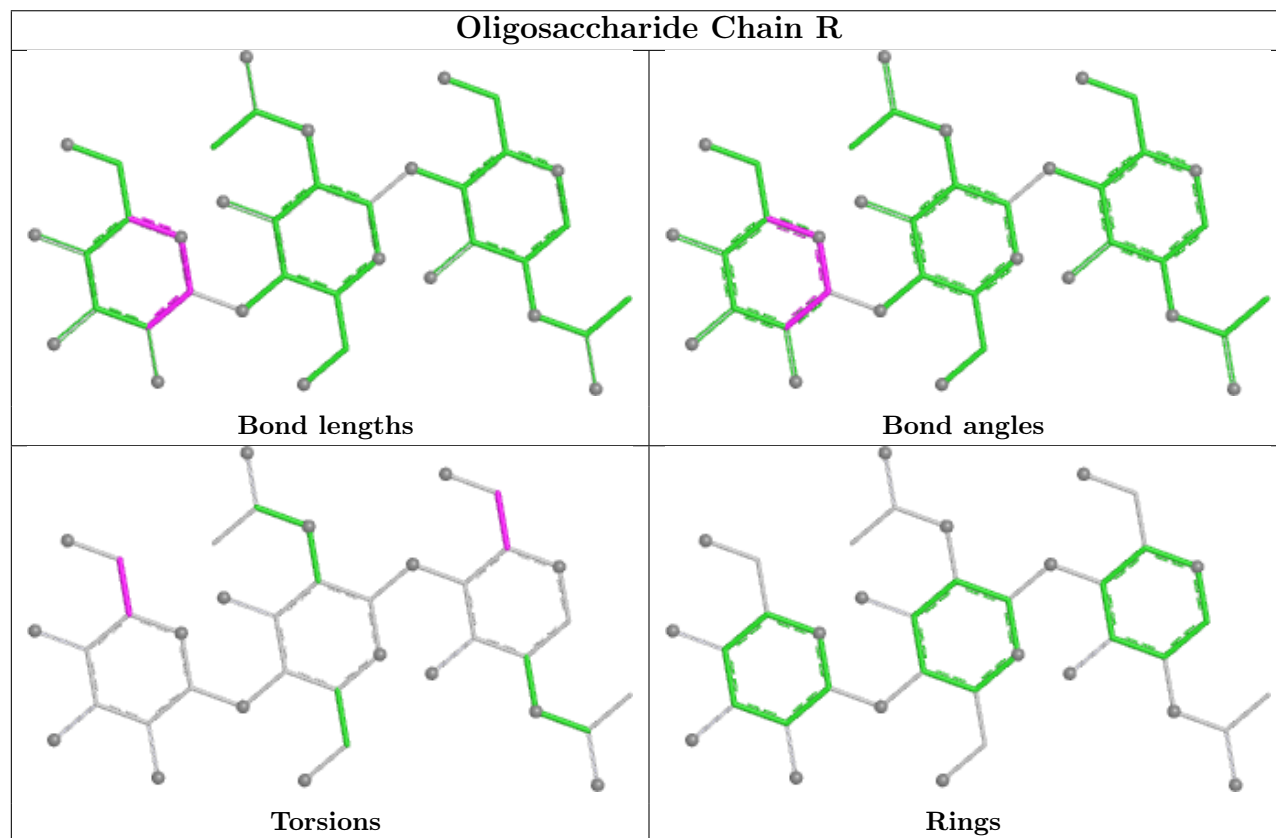
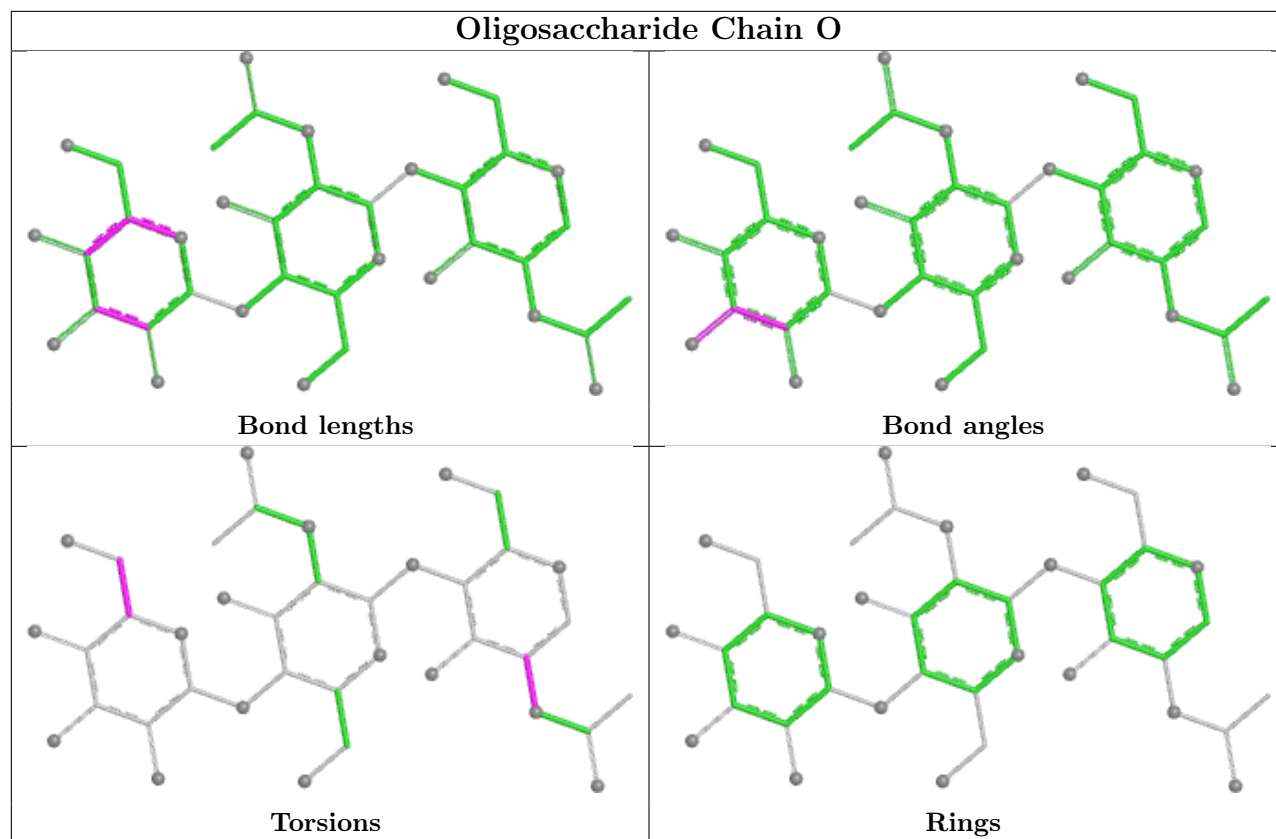


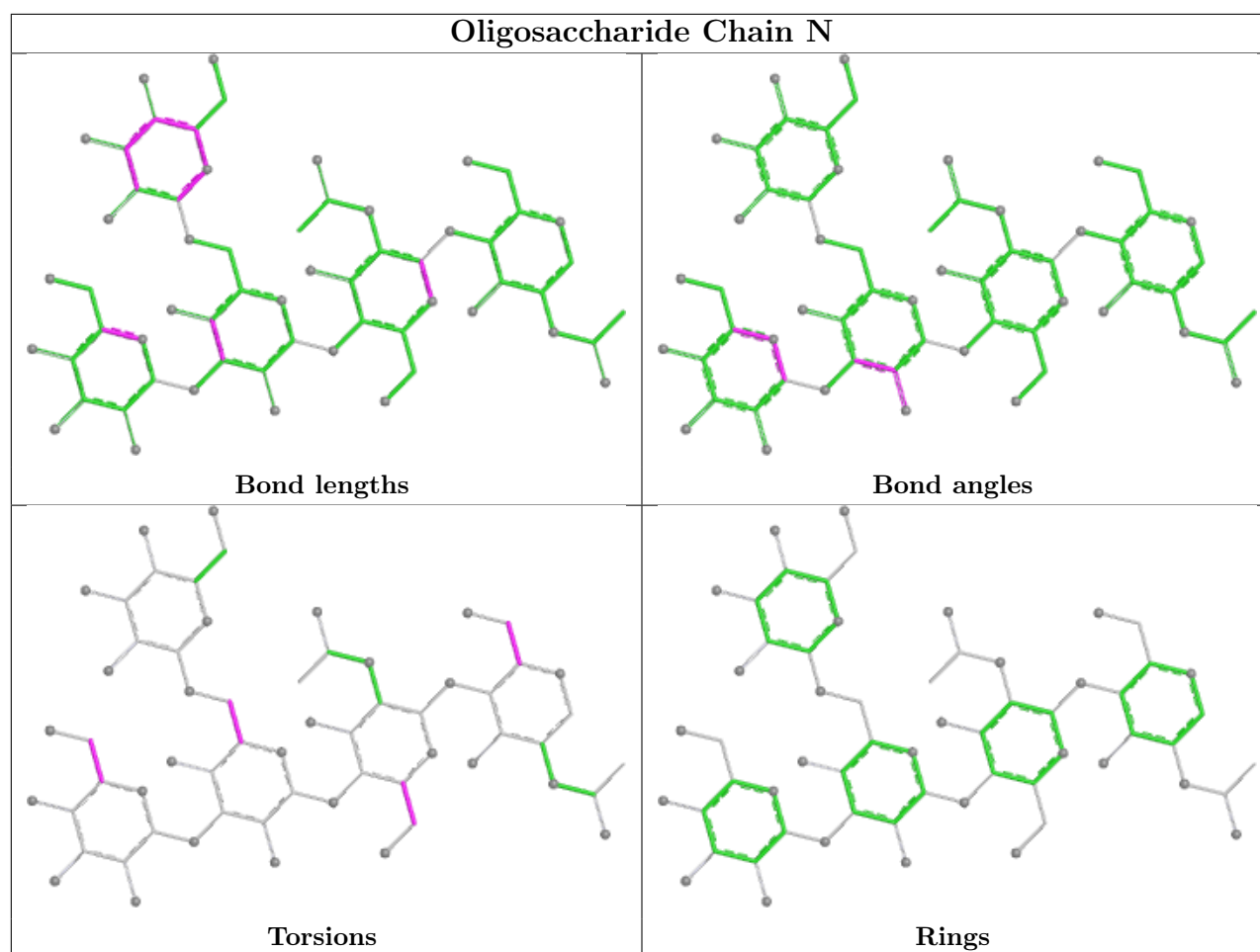












5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 17 are monoatomic - leaving 25 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	B	1002	1	14,14,15	1.09	2 (14%)	17,19,21	0.87	1 (5%)
7	NAG	D	1005	1	14,14,15	0.85	1 (7%)	17,19,21	1.41	2 (11%)
7	NAG	C	1002	1	14,14,15	0.54	0	17,19,21	0.72	0
8	USK	C	1006	6	38,38,38	3.23	18 (47%)	45,53,53	3.91	17 (37%)
7	NAG	A	1005	1	14,14,15	0.62	0	17,19,21	0.58	0
10	EDO	A	1010	-	3,3,3	0.53	0	2,2,2	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	B	1004	1	14,14,15	0.42	0	17,19,21	0.48	0
7	NAG	C	1005	1	14,14,15	0.42	0	17,19,21	0.93	0
7	NAG	D	1004	1	14,14,15	1.01	2 (14%)	17,19,21	0.45	0
7	NAG	B	1003	1	14,14,15	1.40	2 (14%)	17,19,21	1.99	6 (35%)
7	NAG	A	1004	1	14,14,15	0.30	0	17,19,21	0.43	0
7	NAG	D	1002	1	14,14,15	0.72	0	17,19,21	1.38	2 (11%)
7	NAG	A	1007	1	14,14,15	1.08	2 (14%)	17,19,21	0.71	0
9	PGE	A	1009	-	9,9,9	0.37	0	8,8,8	0.74	0
10	EDO	D	1007	-	3,3,3	0.56	0	2,2,2	0.11	0
10	EDO	B	1006	-	3,3,3	0.54	0	2,2,2	0.08	0
7	NAG	A	1006	1	14,14,15	0.86	1 (7%)	17,19,21	0.58	0
7	NAG	C	1003	1	14,14,15	0.78	1 (7%)	17,19,21	0.79	1 (5%)
7	NAG	C	1004	1	14,14,15	0.64	1 (7%)	17,19,21	0.78	1 (5%)
8	USK	A	1008	6	38,38,38	3.30	17 (44%)	45,53,53	3.93	19 (42%)
7	NAG	A	1002	1	14,14,15	0.88	1 (7%)	17,19,21	1.48	2 (11%)
7	NAG	D	1003	1	14,14,15	0.96	1 (7%)	17,19,21	0.52	0
8	USK	B	1005	6	38,38,38	3.23	16 (42%)	45,53,53	3.94	19 (42%)
8	USK	D	1006	6	38,38,38	3.12	16 (42%)	45,53,53	3.67	23 (51%)
7	NAG	A	1003	1	14,14,15	0.85	1 (7%)	17,19,21	1.69	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	1002	1	-	0/6/23/26	0/1/1/1
7	NAG	D	1005	1	-	6/6/23/26	0/1/1/1
7	NAG	C	1002	1	-	0/6/23/26	0/1/1/1
8	USK	C	1006	6	-	7/30/30/30	0/4/4/4
7	NAG	A	1005	1	-	0/6/23/26	0/1/1/1
10	EDO	A	1010	-	-	1/1/1/1	-
7	NAG	B	1004	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1005	1	-	0/6/23/26	0/1/1/1
7	NAG	D	1004	1	-	1/6/23/26	0/1/1/1
7	NAG	B	1003	1	-	3/6/23/26	0/1/1/1
7	NAG	A	1004	1	-	1/6/23/26	0/1/1/1
7	NAG	D	1002	1	-	6/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	1007	1	-	3/6/23/26	0/1/1/1
9	PGE	A	1009	-	-	2/7/7/7	-
10	EDO	D	1007	-	-	1/1/1/1	-
10	EDO	B	1006	-	-	0/1/1/1	-
7	NAG	A	1006	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1003	1	-	3/6/23/26	0/1/1/1
7	NAG	C	1004	1	-	4/6/23/26	0/1/1/1
8	USK	A	1008	6	-	8/30/30/30	0/4/4/4
7	NAG	A	1002	1	-	4/6/23/26	0/1/1/1
7	NAG	D	1003	1	-	4/6/23/26	0/1/1/1
8	USK	B	1005	6	-	13/30/30/30	0/4/4/4
8	USK	D	1006	6	-	10/30/30/30	0/4/4/4
7	NAG	A	1003	1	-	4/6/23/26	0/1/1/1

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1006	USK	C23-N24	11.60	1.45	1.32
8	B	1005	USK	C23-N24	11.48	1.44	1.32
8	D	1006	USK	C23-N24	11.42	1.44	1.32
8	A	1008	USK	C23-N24	11.38	1.44	1.32
8	A	1008	USK	N18-N19	6.16	1.42	1.31
8	B	1005	USK	N18-N19	5.94	1.42	1.31
8	C	1006	USK	N18-N19	5.87	1.42	1.31
8	C	1006	USK	C03-S13	-5.80	1.61	1.71
8	A	1008	USK	C03-S13	-5.80	1.61	1.71
8	B	1005	USK	C15-C16	5.57	1.53	1.49
8	D	1006	USK	C15-C16	5.51	1.53	1.49
8	D	1006	USK	N18-N19	5.49	1.41	1.31
8	D	1006	USK	C03-S13	-5.13	1.62	1.71
8	C	1006	USK	C15-C16	5.08	1.52	1.49
8	B	1005	USK	C03-S13	-4.94	1.63	1.71
8	B	1005	USK	C03-S02	4.77	1.82	1.74
8	B	1005	USK	C22-C21	-4.48	1.46	1.53
8	A	1008	USK	S02-N14	4.40	1.68	1.61
8	A	1008	USK	C08-C07	4.40	1.46	1.39
8	A	1008	USK	C22-C21	-4.38	1.46	1.53
8	B	1005	USK	C08-C07	4.38	1.46	1.39
8	A	1008	USK	C15-C16	4.34	1.52	1.49
8	C	1006	USK	S02-N14	4.30	1.68	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1008	USK	C03-S02	4.28	1.81	1.74
8	C	1006	USK	C05-C04	4.18	1.53	1.39
8	A	1008	USK	C17-C16	4.17	1.42	1.36
8	B	1005	USK	C17-C16	4.12	1.42	1.36
8	A	1008	USK	C05-C04	4.12	1.53	1.39
8	B	1005	USK	S02-N14	4.11	1.67	1.61
8	C	1006	USK	C08-C07	4.11	1.45	1.39
8	B	1005	USK	C05-C04	4.02	1.52	1.39
8	A	1008	USK	O25-N24	-3.99	1.30	1.40
8	C	1006	USK	C17-C16	3.98	1.42	1.36
8	D	1006	USK	C08-C07	3.97	1.45	1.39
8	C	1006	USK	C03-S02	3.90	1.80	1.74
8	D	1006	USK	C03-S02	3.81	1.80	1.74
7	B	1003	NAG	C1-C2	3.79	1.57	1.52
8	D	1006	USK	C17-C16	3.79	1.41	1.36
8	D	1006	USK	C05-C04	3.75	1.51	1.39
8	D	1006	USK	C22-C21	-3.71	1.47	1.53
8	D	1006	USK	S02-N14	3.68	1.67	1.61
8	B	1005	USK	O25-N24	-3.64	1.31	1.40
8	D	1006	USK	O25-N24	-3.63	1.31	1.40
8	C	1006	USK	O25-N24	-3.47	1.31	1.40
7	A	1007	NAG	C1-C2	3.24	1.56	1.52
8	D	1006	USK	C07-C06	3.19	1.53	1.47
8	C	1006	USK	O35-S02	3.18	1.48	1.43
7	B	1002	NAG	O5-C1	3.14	1.49	1.43
8	A	1008	USK	O35-S02	3.14	1.48	1.43
8	C	1006	USK	C22-C21	-3.13	1.48	1.53
8	A	1008	USK	C07-C06	3.08	1.53	1.47
8	B	1005	USK	O35-S02	3.08	1.47	1.43
8	A	1008	USK	O34-C31	2.96	1.43	1.37
7	D	1003	NAG	O5-C1	2.91	1.48	1.43
7	D	1004	NAG	C1-C2	2.87	1.56	1.52
7	D	1005	NAG	C1-C2	2.87	1.56	1.52
8	B	1005	USK	C11-C10	2.78	1.44	1.38
8	D	1006	USK	O35-S02	2.73	1.47	1.43
8	C	1006	USK	C11-C10	2.69	1.44	1.38
8	A	1008	USK	C11-C10	2.65	1.44	1.38
8	A	1008	USK	C06-S13	-2.62	1.62	1.73
7	C	1003	NAG	C1-C2	2.61	1.55	1.52
8	B	1005	USK	C06-S13	-2.60	1.62	1.73
8	C	1006	USK	C06-S13	-2.58	1.62	1.73
8	C	1006	USK	C22-C23	2.46	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1005	USK	C07-C06	2.45	1.52	1.47
8	D	1006	USK	O34-C31	2.45	1.42	1.37
7	A	1006	NAG	C1-C2	2.44	1.55	1.52
7	A	1002	NAG	C1-C2	2.44	1.55	1.52
8	C	1006	USK	O34-C31	2.40	1.42	1.37
7	A	1003	NAG	O5-C1	2.36	1.47	1.43
7	B	1002	NAG	C1-C2	2.35	1.55	1.52
7	B	1003	NAG	C3-C2	2.26	1.57	1.52
8	B	1005	USK	O34-C31	2.22	1.42	1.37
7	D	1004	NAG	O5-C1	2.21	1.47	1.43
8	D	1006	USK	C06-S13	-2.20	1.63	1.73
8	C	1006	USK	C07-C06	2.19	1.51	1.47
8	A	1008	USK	C30-C31	2.15	1.43	1.39
8	C	1006	USK	C33-C28	2.15	1.43	1.38
8	D	1006	USK	C11-C10	2.15	1.43	1.38
7	C	1004	NAG	O5-C1	2.07	1.47	1.43
7	A	1007	NAG	O5-C1	2.00	1.47	1.43

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1008	USK	C03-S13-C06	15.21	103.91	90.41
8	B	1005	USK	C03-S13-C06	14.43	103.21	90.41
8	C	1006	USK	C03-S13-C06	13.91	102.75	90.41
8	D	1006	USK	C03-S13-C06	12.76	101.73	90.41
8	C	1006	USK	C15-C16-C17	-12.01	119.88	131.48
8	C	1006	USK	O35-S02-O01	-10.67	100.26	119.82
8	B	1005	USK	C15-C16-C17	-10.62	121.22	131.48
8	B	1005	USK	O35-S02-O01	-10.59	100.41	119.82
8	A	1008	USK	C15-C16-C17	-10.58	121.26	131.48
8	D	1006	USK	O35-S02-O01	-10.24	101.05	119.82
8	A	1008	USK	O35-S02-O01	-9.90	101.66	119.82
8	D	1006	USK	C15-C16-C17	-7.81	123.93	131.48
8	A	1008	USK	O01-S02-N14	6.82	113.79	107.41
8	D	1006	USK	C15-N14-S02	-6.15	106.88	119.78
8	B	1005	USK	O35-S02-C03	5.92	114.33	107.21
8	A	1008	USK	C16-N20-N19	-5.39	106.98	111.15
8	D	1006	USK	O01-S02-N14	5.21	112.28	107.41
8	B	1005	USK	C04-C03-S13	-5.20	107.38	112.55
8	C	1006	USK	O26-C23-N24	-5.09	117.02	123.27
8	C	1006	USK	O01-S02-N14	4.91	112.00	107.41
8	B	1005	USK	O01-S02-C03	4.71	112.88	107.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1006	USK	O35-S02-C03	4.71	112.88	107.21
8	D	1006	USK	O35-S02-N14	4.71	111.81	107.41
8	A	1008	USK	C04-C03-S13	-4.66	107.92	112.55
7	A	1002	NAG	C2-N2-C7	4.65	129.13	122.90
8	C	1006	USK	C16-N20-N19	-4.62	107.57	111.15
8	C	1006	USK	O35-S02-N14	4.55	111.66	107.41
8	A	1008	USK	O01-S02-C03	4.46	112.58	107.21
7	D	1002	NAG	C2-N2-C7	4.45	128.86	122.90
8	D	1006	USK	O35-S02-C03	4.43	112.55	107.21
7	A	1003	NAG	C2-N2-C7	4.42	128.82	122.90
7	D	1005	NAG	C2-N2-C7	4.39	128.78	122.90
8	D	1006	USK	O26-C23-N24	-4.36	117.92	123.27
8	B	1005	USK	C16-N20-N19	-4.33	107.80	111.15
8	C	1006	USK	C04-C03-S13	-4.28	108.29	112.55
8	B	1005	USK	O26-C23-N24	-4.23	118.08	123.27
7	B	1003	NAG	C2-N2-C7	4.19	128.52	122.90
8	B	1005	USK	O01-S02-N14	4.16	111.29	107.41
8	A	1008	USK	O35-S02-C03	4.05	112.09	107.21
8	B	1005	USK	S13-C03-S02	4.01	125.66	120.43
8	D	1006	USK	C22-C23-N24	3.93	121.09	115.14
8	C	1006	USK	N20-N19-N18	3.87	109.66	106.94
8	A	1008	USK	N20-N19-N18	3.87	109.65	106.94
8	B	1005	USK	C22-C23-N24	3.84	120.96	115.14
8	B	1005	USK	C15-N14-S02	-3.77	111.87	119.78
8	A	1008	USK	C17-C16-N20	3.70	108.30	103.81
7	B	1003	NAG	C1-C2-N2	3.69	116.25	110.43
8	C	1006	USK	C04-C05-C06	-3.60	109.02	113.58
8	A	1008	USK	C15-N14-S02	-3.57	112.29	119.78
8	D	1006	USK	S13-C03-S02	3.54	125.04	120.43
8	B	1005	USK	N20-N19-N18	3.50	109.40	106.94
8	D	1006	USK	C04-C03-S13	-3.48	109.08	112.55
8	C	1006	USK	C22-C23-N24	3.44	120.34	115.14
8	C	1006	USK	C15-N14-S02	-3.40	112.64	119.78
7	B	1003	NAG	C4-C3-C2	3.31	115.86	111.02
8	D	1006	USK	C16-N20-N19	-3.27	108.62	111.15
7	A	1003	NAG	C1-C2-N2	3.21	115.50	110.43
7	B	1003	NAG	C3-C4-C5	3.08	115.82	110.23
8	B	1005	USK	C17-C16-N20	3.06	107.51	103.81
7	B	1002	NAG	C1-O5-C5	3.05	116.28	112.19
8	C	1006	USK	O01-S02-C03	3.03	110.86	107.21
8	A	1008	USK	O35-S02-N14	3.03	110.24	107.41
8	A	1008	USK	C28-C27-C21	3.03	119.07	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1005	USK	C04-C05-C06	-2.99	109.79	113.58
8	D	1006	USK	O01-S02-C03	2.97	110.79	107.21
8	C	1006	USK	C28-C27-C21	2.95	118.92	113.22
7	A	1003	NAG	C1-O5-C5	2.92	116.10	112.19
8	D	1006	USK	C11-C12-C07	2.92	123.24	120.36
8	D	1006	USK	C28-C27-C21	2.88	118.79	113.22
8	D	1006	USK	C17-C16-N20	2.87	107.29	103.81
8	C	1006	USK	C17-C16-N20	2.85	107.27	103.81
8	D	1006	USK	C21-N20-N19	2.84	123.90	120.39
7	D	1005	NAG	C1-O5-C5	2.84	115.99	112.19
8	B	1005	USK	C32-C33-C28	-2.79	117.33	121.00
8	D	1006	USK	C04-C05-C06	-2.69	110.17	113.58
8	B	1005	USK	O35-S02-N14	2.61	109.85	107.41
7	C	1003	NAG	C1-O5-C5	2.59	115.66	112.19
7	B	1003	NAG	O4-C4-C5	-2.57	103.00	109.32
7	A	1002	NAG	C1-C2-N2	2.56	114.47	110.43
8	A	1008	USK	C04-C05-C06	-2.53	110.38	113.58
8	C	1006	USK	C17-N18-N19	-2.52	106.31	108.80
7	C	1004	NAG	C1-O5-C5	2.49	115.53	112.19
8	D	1006	USK	C07-C06-S13	2.38	127.08	121.02
8	D	1006	USK	C10-C11-C12	-2.37	117.31	120.24
8	D	1006	USK	C07-C06-C05	-2.35	124.08	128.47
8	A	1008	USK	C21-N20-N19	2.34	123.29	120.39
8	D	1006	USK	N20-N19-N18	2.32	108.57	106.94
8	B	1005	USK	C33-C28-C29	2.25	121.58	118.23
8	A	1008	USK	C27-C28-C33	-2.22	116.77	120.90
8	D	1006	USK	O25-N24-C23	-2.20	116.55	119.79
8	A	1008	USK	C05-C06-S13	-2.17	107.78	110.10
7	D	1002	NAG	C1-C2-N2	2.17	113.85	110.43
7	B	1003	NAG	C1-O5-C5	-2.14	109.32	112.19
8	A	1008	USK	C17-N18-N19	-2.11	106.72	108.80
8	B	1005	USK	C17-N18-N19	-2.09	106.73	108.80
8	A	1008	USK	C05-C04-C03	-2.08	110.01	112.34

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1003	NAG	C3-C2-N2-C7
7	B	1003	NAG	C1-C2-N2-C7
8	A	1008	USK	C05-C06-C07-C08
8	A	1008	USK	C05-C06-C07-C12

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Mol	Chain	Res	Type	Atoms
8	A	1008	USK	S13-C06-C07-C08
8	B	1005	USK	C22-C21-C27-C28
8	B	1005	USK	S13-C03-S02-O35
8	B	1005	USK	C05-C06-C07-C08
8	B	1005	USK	C05-C06-C07-C12
8	B	1005	USK	S13-C06-C07-C08
8	B	1005	USK	S13-C06-C07-C12
8	C	1006	USK	C04-C03-S02-O01
8	C	1006	USK	S13-C03-S02-O01
8	D	1006	USK	C05-C06-C07-C08
8	D	1006	USK	C05-C06-C07-C12
8	D	1006	USK	S13-C06-C07-C08
8	D	1006	USK	S13-C06-C07-C12
8	A	1008	USK	S13-C06-C07-C12
7	D	1002	NAG	O5-C5-C6-O6
7	B	1004	NAG	O5-C5-C6-O6
7	D	1002	NAG	C4-C5-C6-O6
7	B	1004	NAG	C4-C5-C6-O6
7	D	1005	NAG	O5-C5-C6-O6
7	A	1002	NAG	C8-C7-N2-C2
7	A	1002	NAG	O7-C7-N2-C2
7	C	1003	NAG	C8-C7-N2-C2
7	C	1003	NAG	O7-C7-N2-C2
7	C	1004	NAG	C8-C7-N2-C2
7	C	1004	NAG	O7-C7-N2-C2
7	D	1002	NAG	C8-C7-N2-C2
7	D	1002	NAG	O7-C7-N2-C2
7	D	1003	NAG	C8-C7-N2-C2
7	D	1003	NAG	O7-C7-N2-C2
7	D	1005	NAG	C8-C7-N2-C2
7	D	1005	NAG	O7-C7-N2-C2
7	D	1003	NAG	O5-C5-C6-O6
7	D	1005	NAG	C4-C5-C6-O6
7	C	1003	NAG	O5-C5-C6-O6
7	A	1006	NAG	O5-C5-C6-O6
7	A	1003	NAG	O5-C5-C6-O6
7	B	1003	NAG	C4-C5-C6-O6
8	B	1005	USK	C15-N14-S02-O01
7	C	1004	NAG	C4-C5-C6-O6
10	D	1007	EDO	O1-C1-C2-O2
7	A	1007	NAG	C4-C5-C6-O6
7	A	1004	NAG	O5-C5-C6-O6

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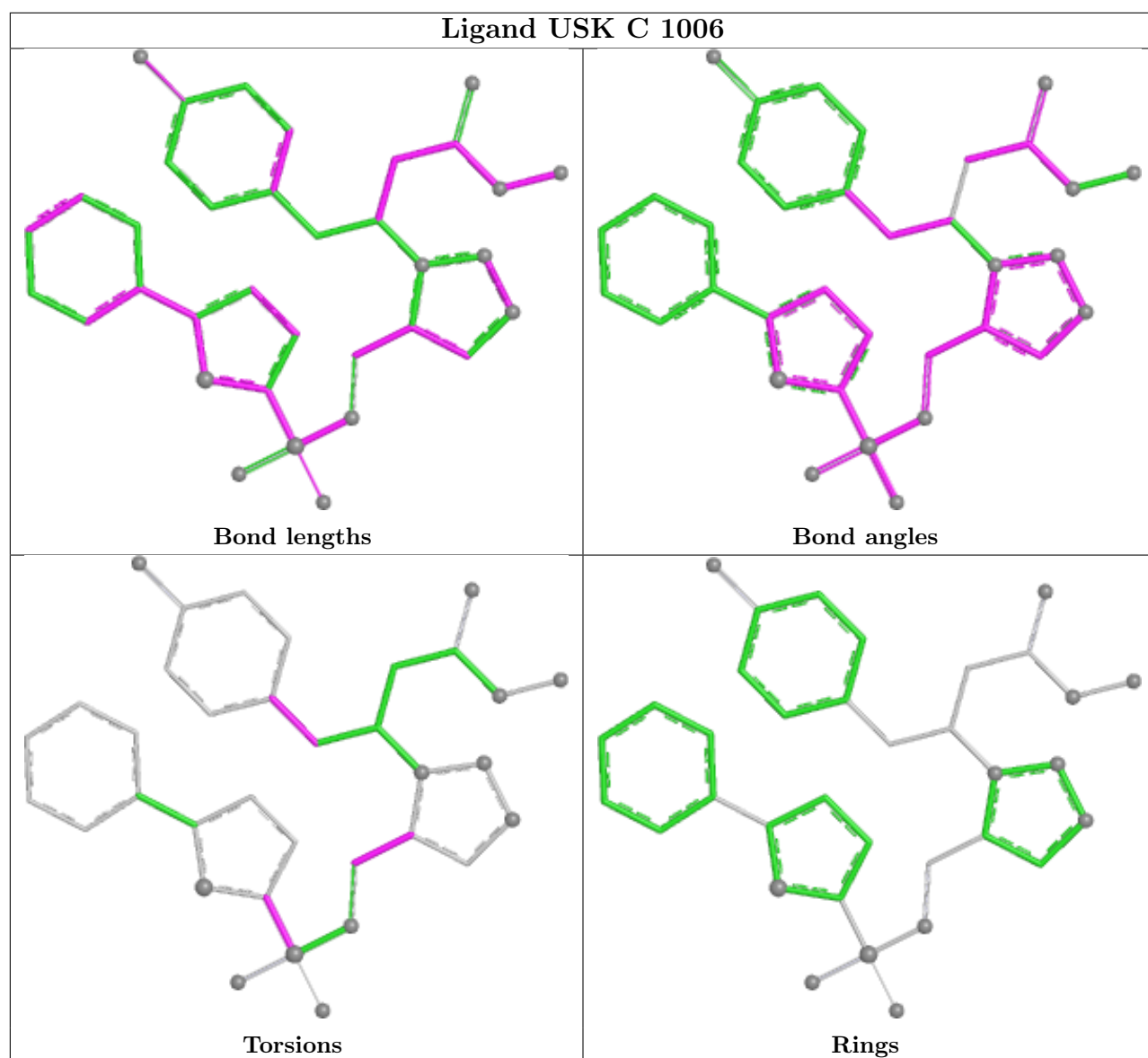
Mol	Chain	Res	Type	Atoms
7	A	1002	NAG	O5-C5-C6-O6
7	D	1004	NAG	O5-C5-C6-O6
7	D	1003	NAG	C4-C5-C6-O6
7	A	1007	NAG	O5-C5-C6-O6
7	C	1004	NAG	O5-C5-C6-O6
8	B	1005	USK	C21-C27-C28-C29
8	A	1008	USK	S13-C03-S02-O35
8	B	1005	USK	C04-C03-S02-O35
8	D	1006	USK	C04-C03-S02-O01
8	D	1006	USK	S13-C03-S02-O01
8	B	1005	USK	C21-C27-C28-C33
8	D	1006	USK	C15-N14-S02-O35
8	C	1006	USK	C21-C27-C28-C33
8	C	1006	USK	C21-C27-C28-C29
7	B	1003	NAG	O5-C5-C6-O6
9	A	1009	PGE	O3-C5-C6-O4
7	A	1002	NAG	C3-C2-N2-C7
7	A	1007	NAG	C3-C2-N2-C7
7	D	1002	NAG	C3-C2-N2-C7
8	B	1005	USK	S13-C03-S02-N14
8	C	1006	USK	N14-C15-C16-N20
8	C	1006	USK	S13-C03-S02-N14
8	D	1006	USK	N14-C15-C16-N20
8	D	1006	USK	S13-C03-S02-N14
8	B	1005	USK	C15-N14-S02-C03
7	A	1006	NAG	C4-C5-C6-O6
8	B	1005	USK	C04-C03-S02-N14
8	C	1006	USK	C04-C03-S02-N14
8	A	1008	USK	C04-C03-S02-O35
7	A	1003	NAG	C4-C5-C6-O6
8	A	1008	USK	C21-C27-C28-C29
8	A	1008	USK	C21-C27-C28-C33
7	A	1003	NAG	C1-C2-N2-C7
7	D	1002	NAG	C1-C2-N2-C7
7	D	1005	NAG	C1-C2-N2-C7
10	A	1010	EDO	O1-C1-C2-O2
7	D	1005	NAG	C3-C2-N2-C7
9	A	1009	PGE	O2-C3-C4-O3
8	D	1006	USK	C16-C15-N14-S02

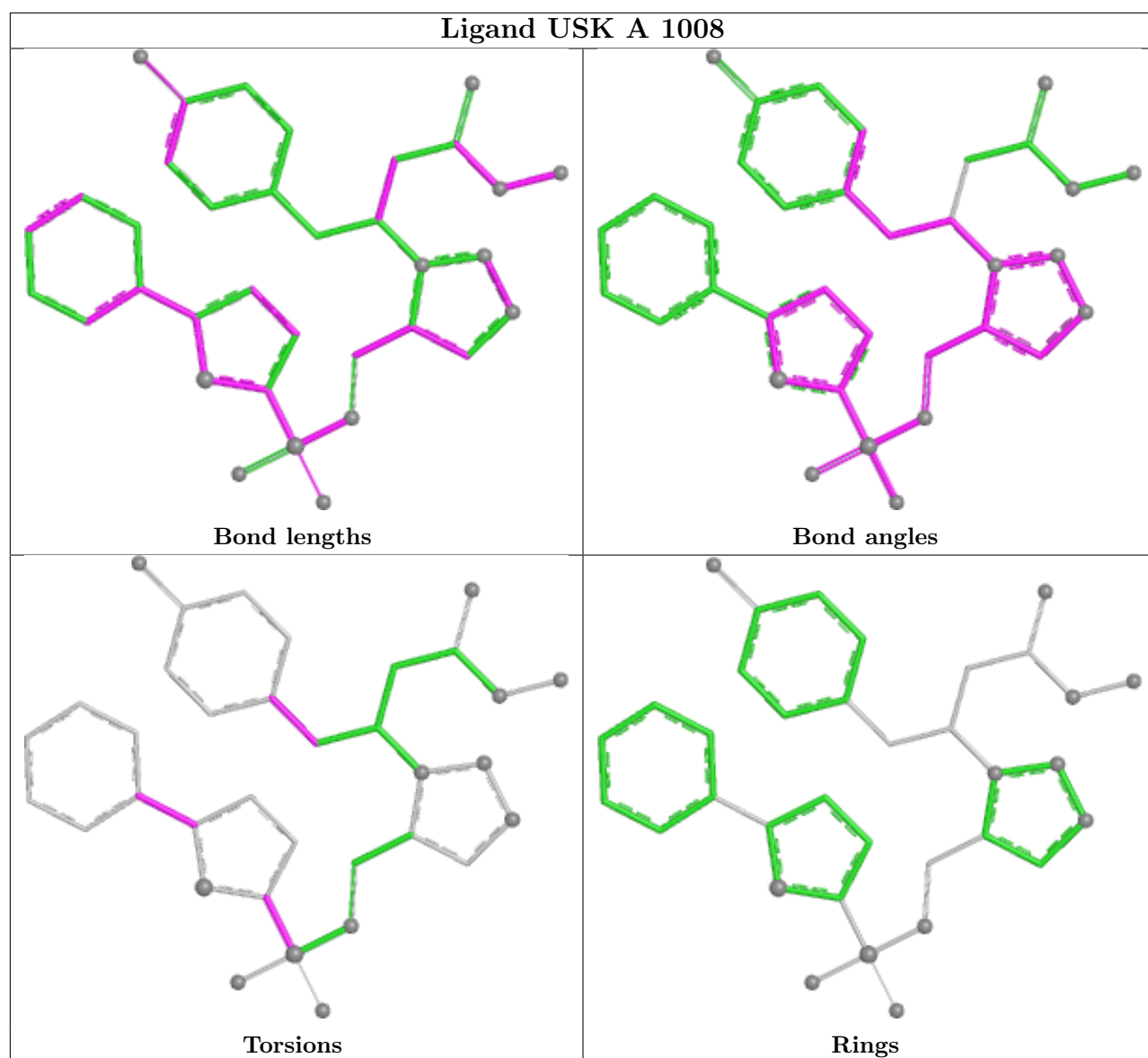
There are no ring outliers.

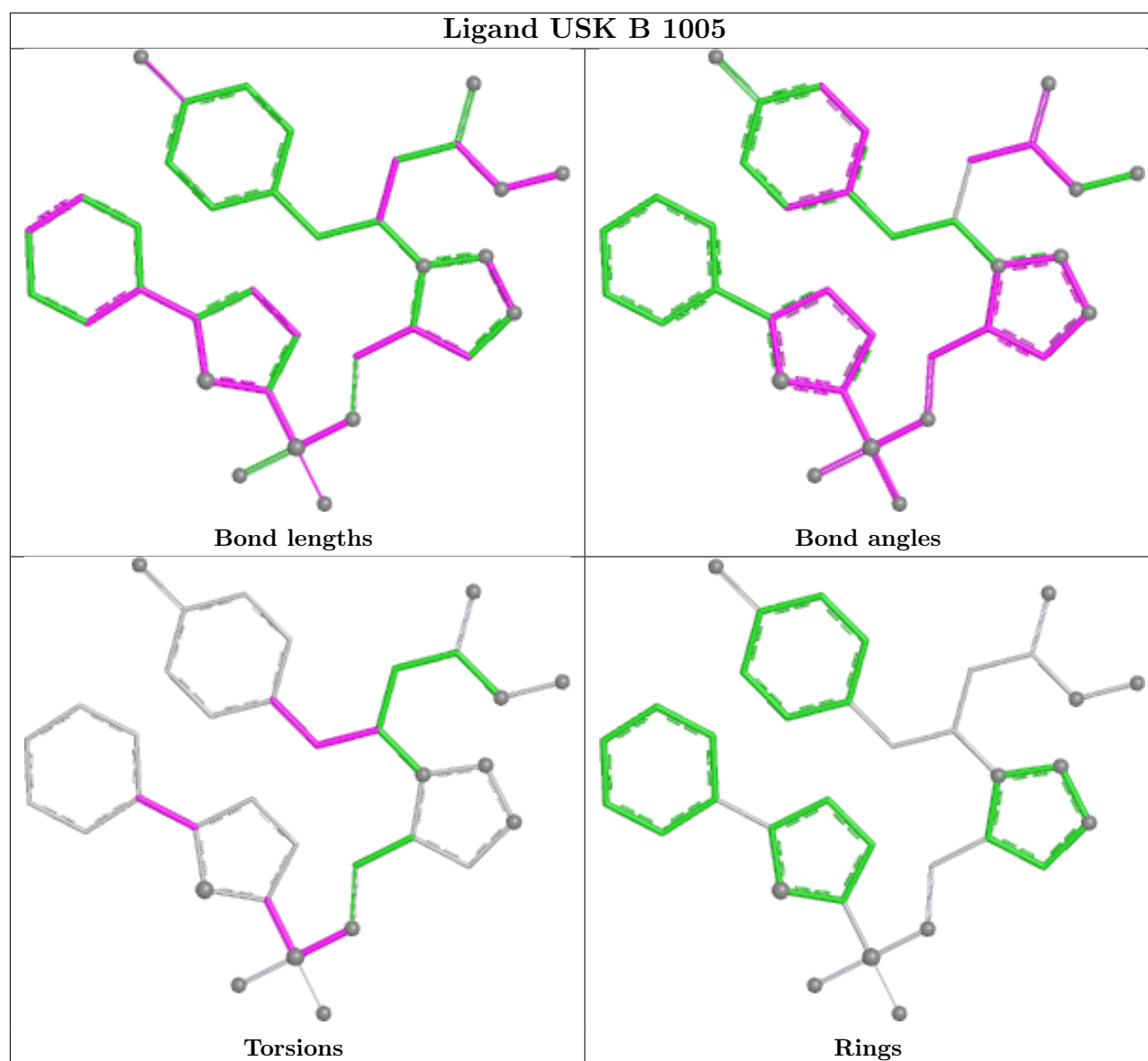
8 monomers are involved in 10 short contacts:

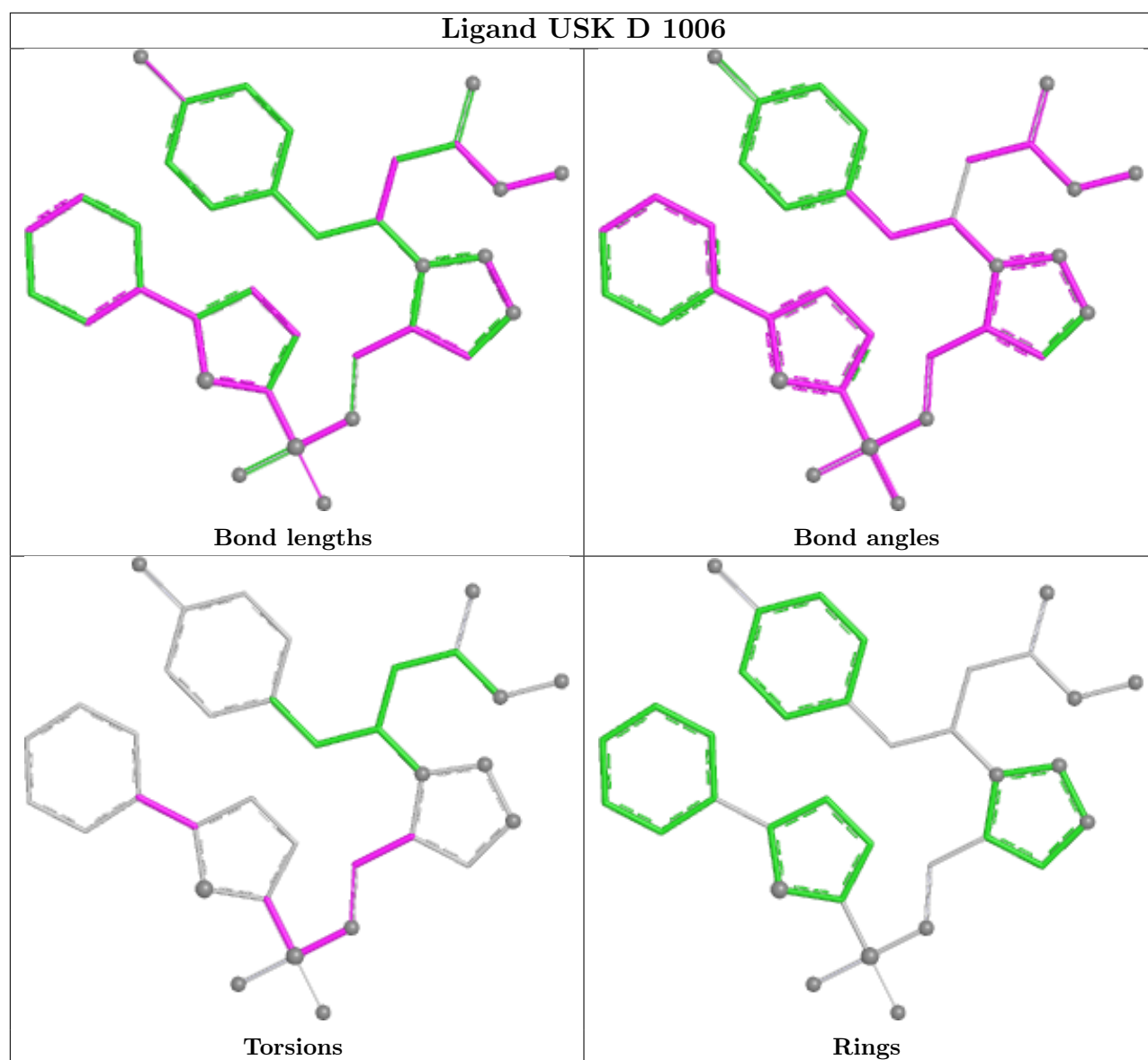
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1002	NAG	1	0
7	D	1005	NAG	1	0
8	C	1006	USK	2	0
7	B	1004	NAG	1	0
7	D	1002	NAG	1	0
7	A	1002	NAG	1	0
8	B	1005	USK	2	0
8	D	1006	USK	1	0

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

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	915/966 (94%)	-1.42	0 100 100	15, 37, 80, 133	2 (0%)
1	B	907/966 (93%)	-1.30	0 100 100	18, 46, 88, 152	3 (0%)
1	C	883/966 (91%)	-1.16	0 100 100	24, 60, 107, 154	0
1	D	884/966 (91%)	-1.06	0 100 100	25, 66, 116, 159	3 (0%)
All	All	3589/3864 (92%)	-1.24	0 100 100	15, 51, 103, 159	8 (0%)

There are no RSRZ outliers to report.

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	M	2	14/15	0.92	0.09	65,117,124,126	0
3	NAG	K	2	14/15	0.93	0.07	96,111,115,117	0
3	NAG	J	2	14/15	0.93	0.09	79,93,106,107	0
3	NAG	M	1	14/15	0.94	0.08	80,101,116,122	0
2	BMA	E	3	11/12	0.95	0.06	75,79,89,89	0
2	BMA	Q	3	11/12	0.95	0.06	61,78,83,96	0
4	BMA	I	3	11/12	0.95	0.07	79,95,103,104	0
3	NAG	S	1	14/15	0.96	0.07	57,78,107,109	0
3	NAG	G	2	14/15	0.96	0.05	62,81,88,97	0

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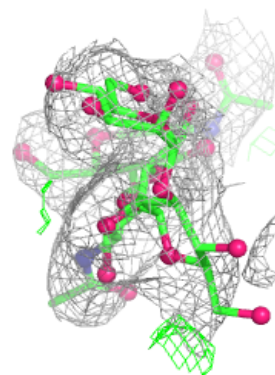
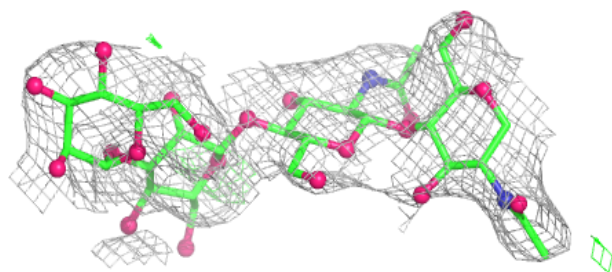
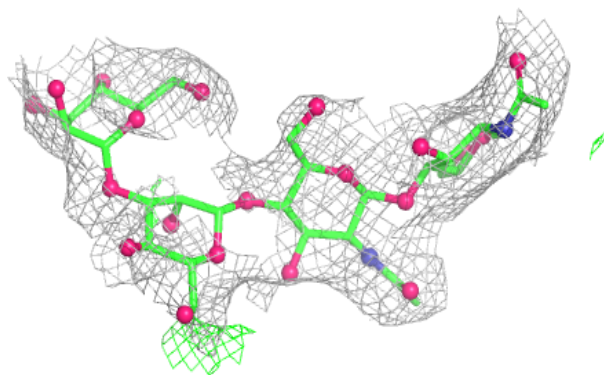
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MAN	E	4	11/12	0.97	0.05	77,94,100,113	0
2	MAN	Q	4	11/12	0.97	0.05	60,72,89,94	0
3	NAG	P	2	14/15	0.97	0.06	89,111,120,122	0
3	NAG	K	1	14/15	0.97	0.04	67,85,109,115	0
3	NAG	S	2	14/15	0.97	0.07	55,102,111,114	0
4	BMA	H	3	11/12	0.97	0.06	90,98,103,103	0
3	NAG	F	2	14/15	0.97	0.05	20,46,67,67	0
4	NAG	O	2	14/15	0.97	0.05	52,79,100,102	0
4	BMA	O	3	11/12	0.97	0.06	59,75,95,96	0
4	NAG	R	2	14/15	0.97	0.07	55,86,100,104	0
4	BMA	R	3	11/12	0.97	0.07	89,100,112,118	0
5	BMA	N	3	11/12	0.97	0.06	60,72,82,83	0
5	MAN	N	4	11/12	0.97	0.06	38,60,85,97	0
4	NAG	O	1	14/15	0.98	0.07	55,77,93,102	0
3	NAG	G	1	14/15	0.98	0.05	39,55,75,83	0
2	NAG	Q	2	14/15	0.98	0.05	56,77,81,89	0
3	NAG	L	1	14/15	0.98	0.05	64,86,91,98	0
4	NAG	H	2	14/15	0.98	0.05	73,82,92,100	0
5	NAG	N	2	14/15	0.98	0.04	39,53,76,81	0
3	NAG	J	1	14/15	0.98	0.05	48,65,81,101	0
2	NAG	E	2	14/15	0.98	0.05	44,74,92,93	0
5	MAN	N	5	11/12	0.98	0.05	67,85,90,92	0
3	NAG	F	1	14/15	0.99	0.03	14,36,44,47	0
4	NAG	H	1	14/15	0.99	0.04	44,53,69,76	0
4	NAG	R	1	14/15	0.99	0.04	39,62,69,79	0
2	NAG	Q	1	14/15	0.99	0.04	35,52,76,79	0
3	NAG	P	1	14/15	0.99	0.05	57,76,104,114	0
5	NAG	N	1	14/15	0.99	0.04	30,41,55,68	0
4	NAG	I	1	14/15	0.99	0.07	23,37,46,51	0
4	NAG	I	2	14/15	0.99	0.04	26,57,76,84	0
2	NAG	E	1	14/15	0.99	0.05	27,40,59,64	0
3	NAG	L	2	14/15	0.99	0.06	87,101,109,111	0

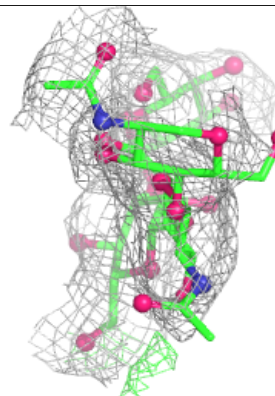
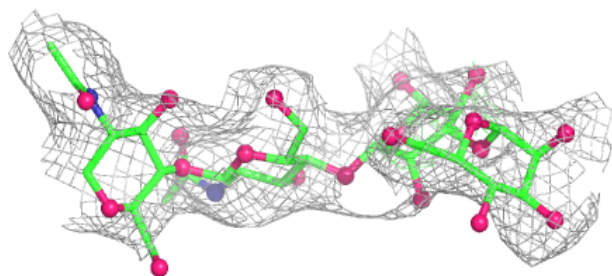
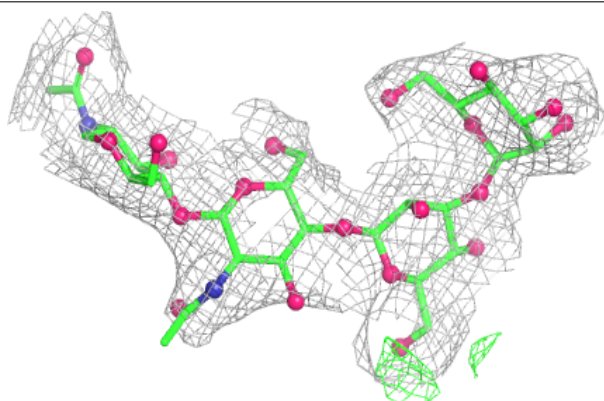
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

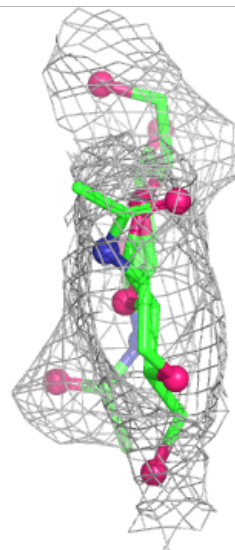
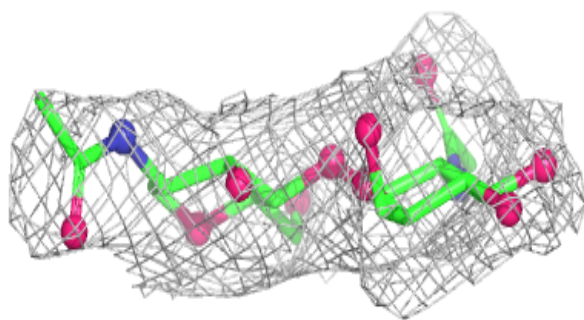
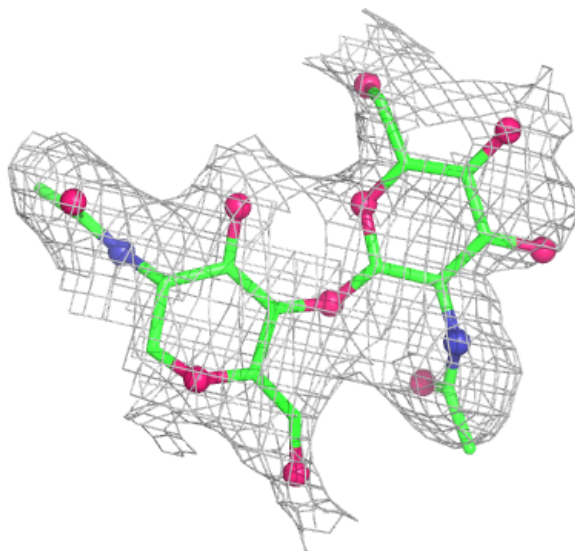
**Electron density around Chain Q:**

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



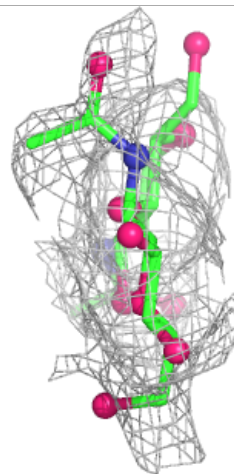
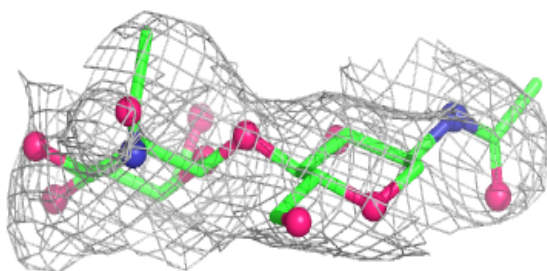
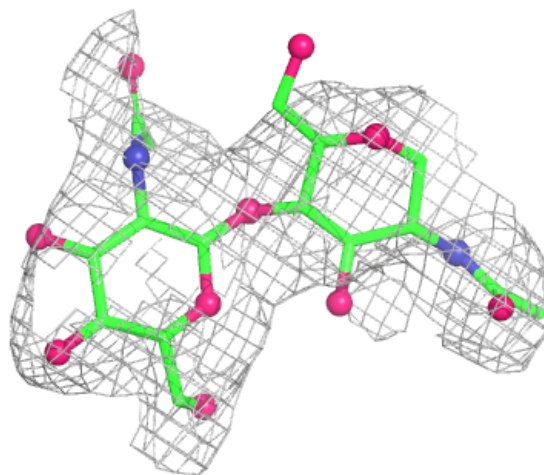
Electron density around Chain F:

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



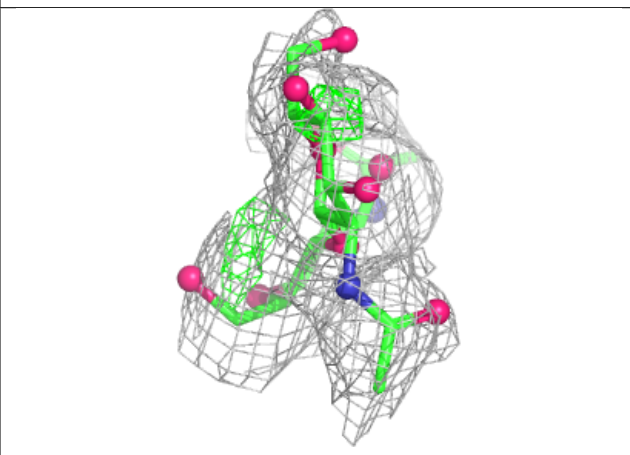
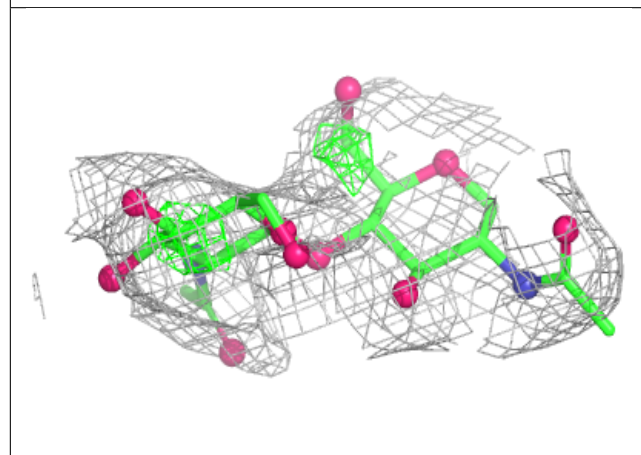
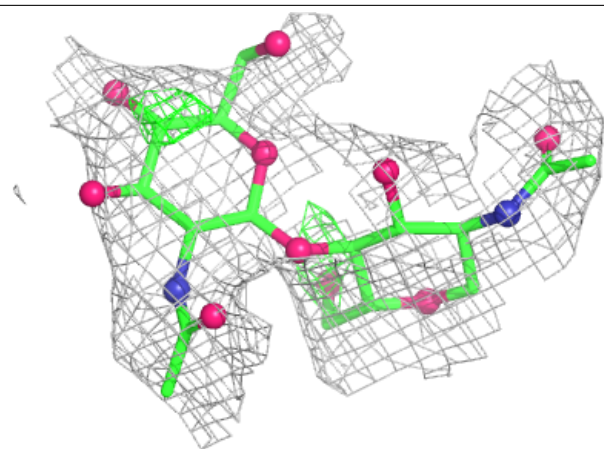
Electron density around Chain G:

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



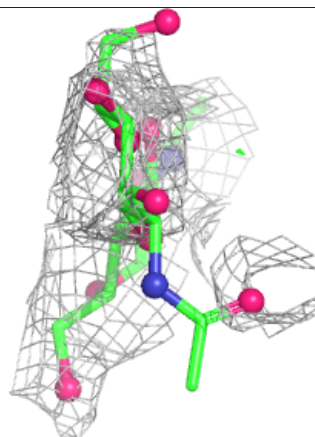
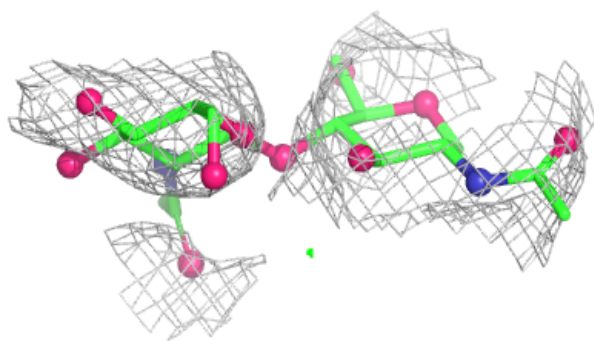
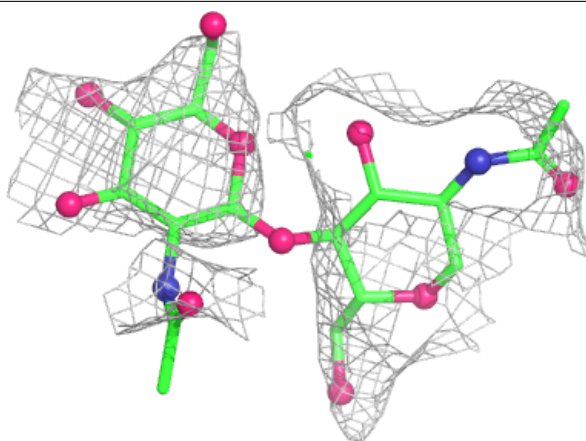
Electron density around Chain J:

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



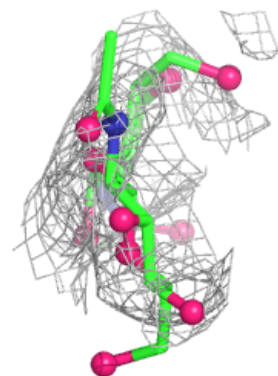
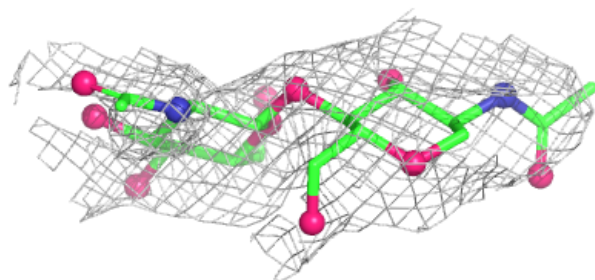
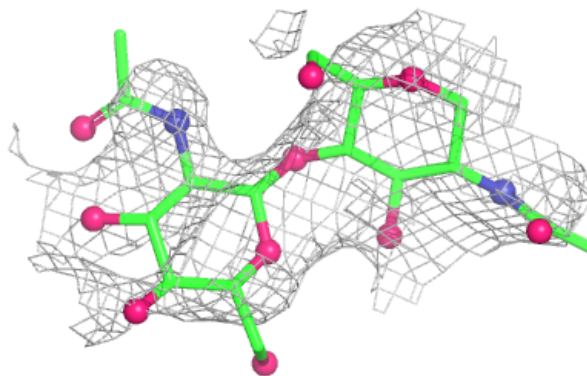
Electron density around Chain K:

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



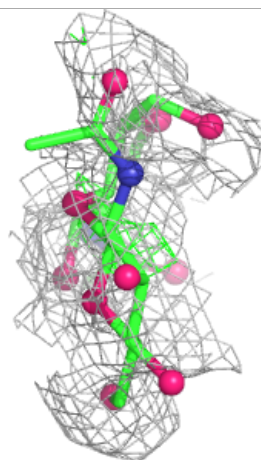
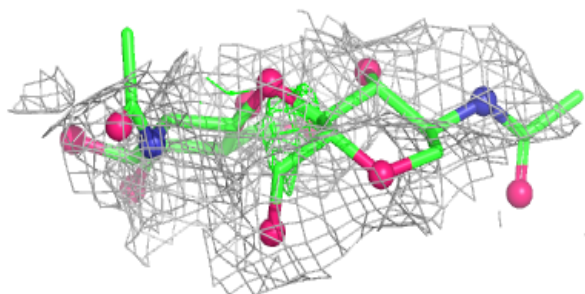
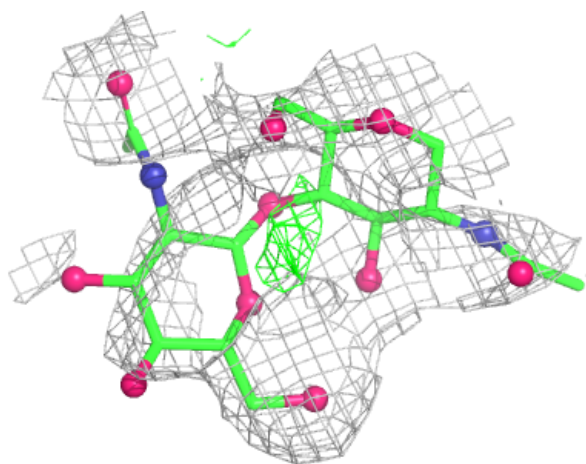
Electron density around Chain L:

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



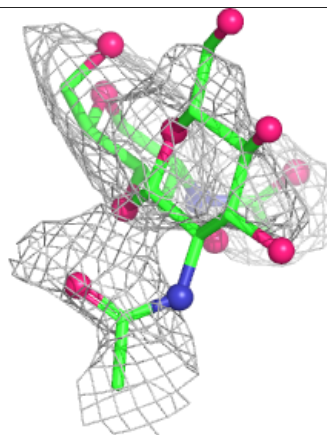
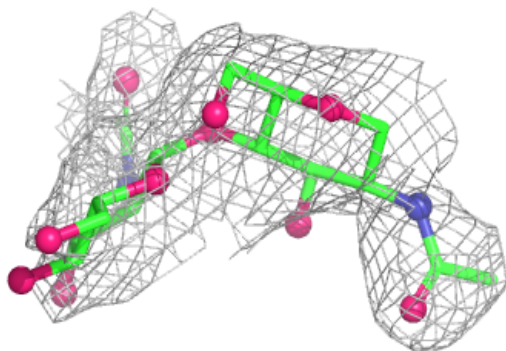
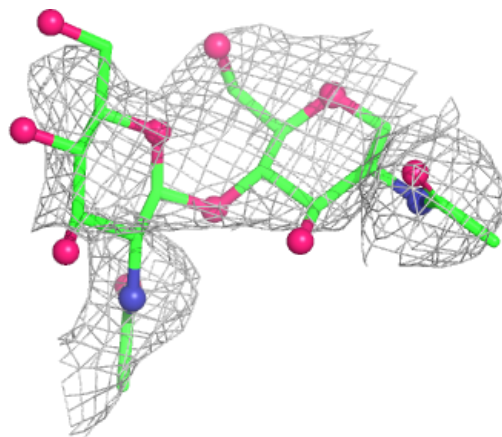
Electron density around Chain M:

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



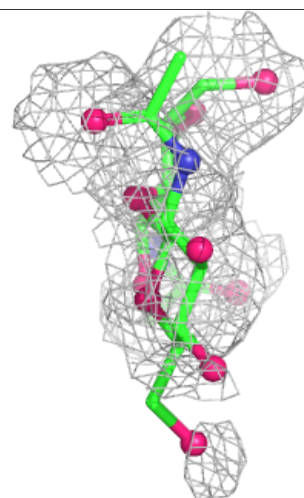
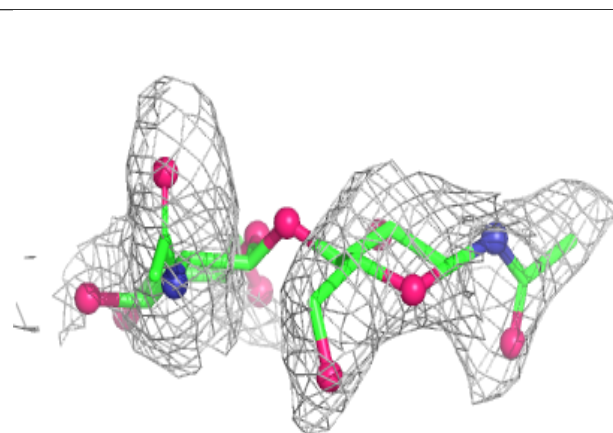
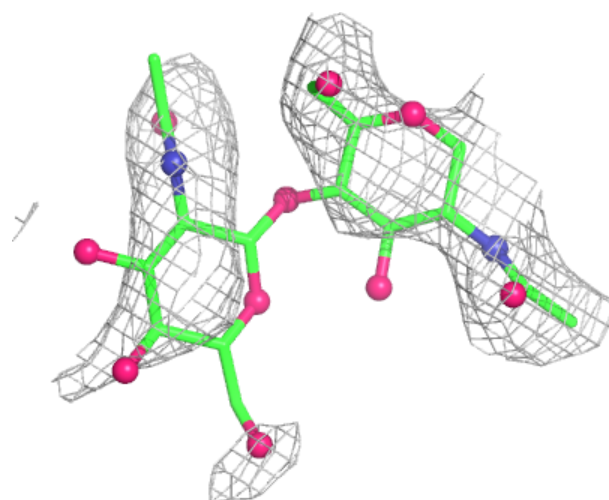
Electron density around Chain P:

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



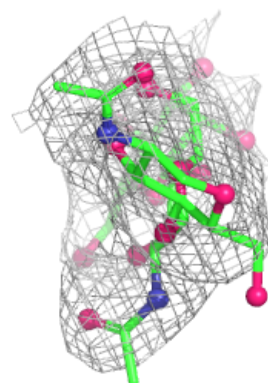
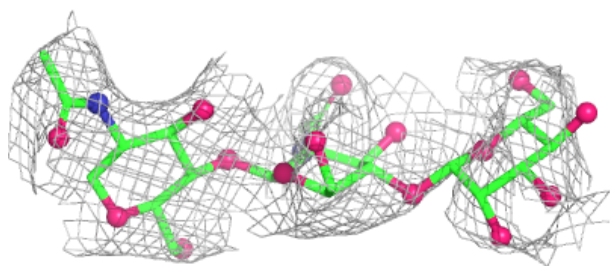
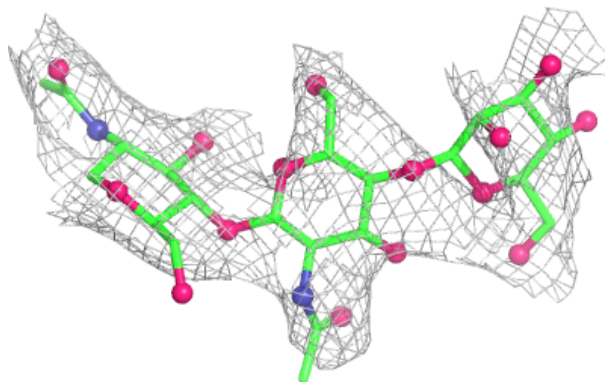
Electron density around Chain S:

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

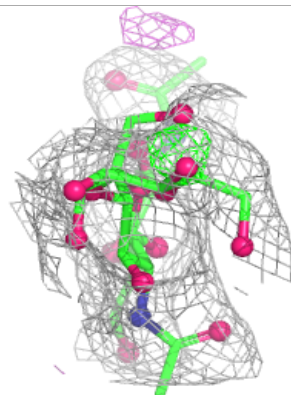
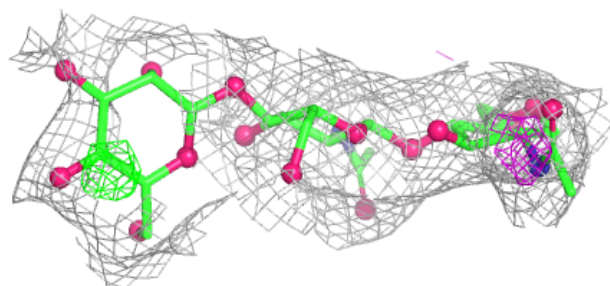
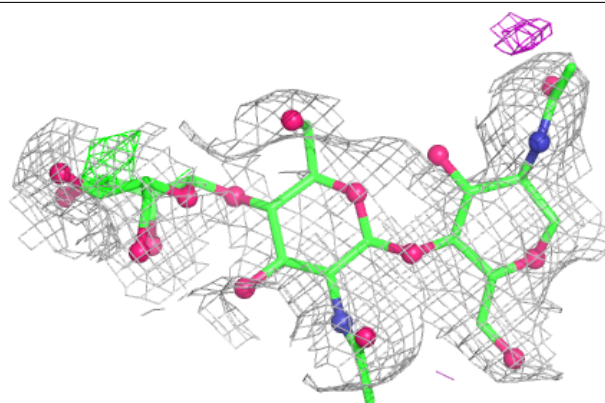


Electron density around Chain H:

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

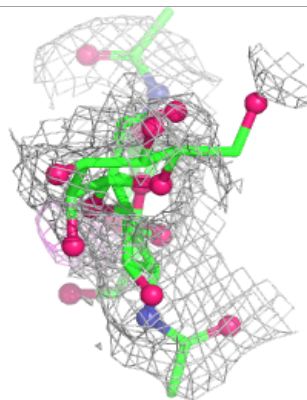
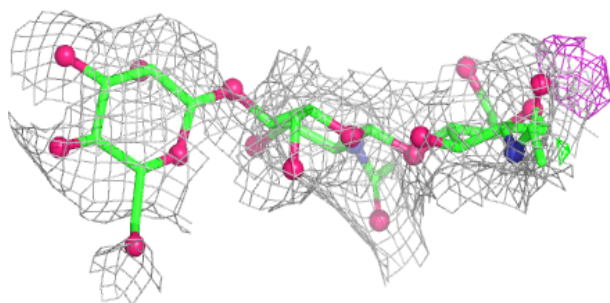
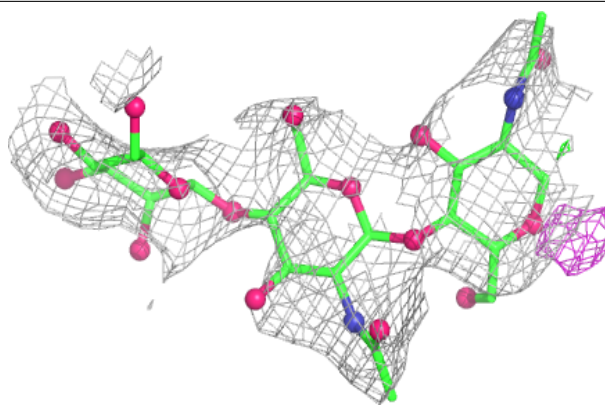
**Electron density around Chain I:**

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

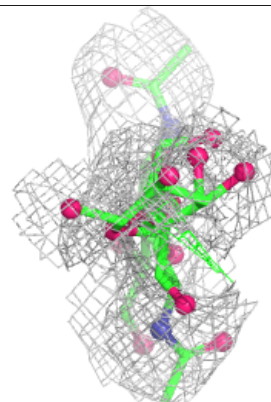
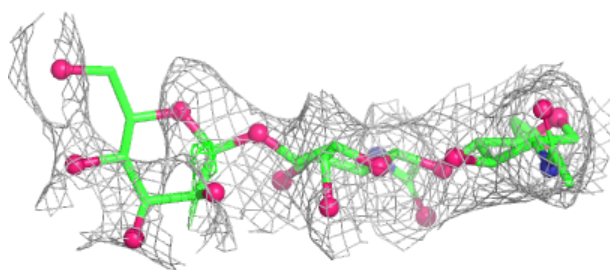
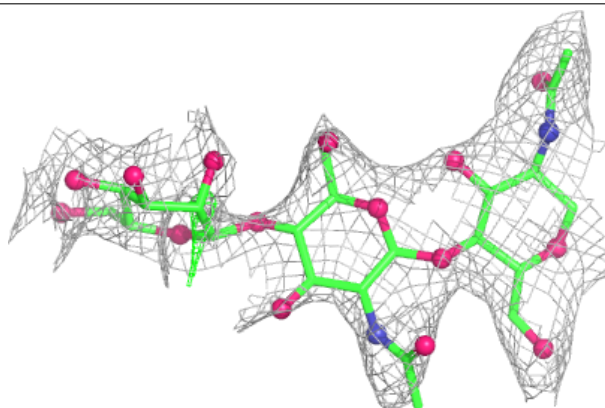


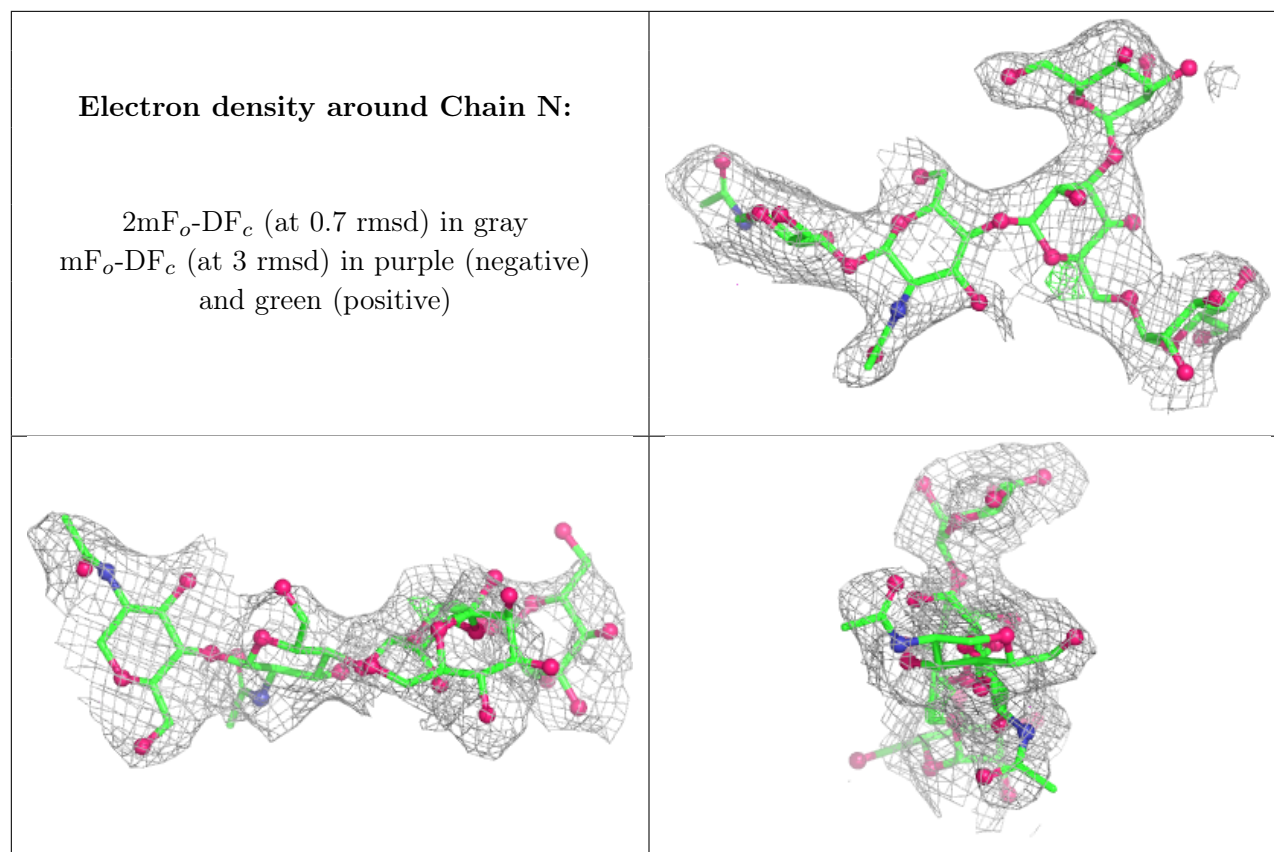
Electron density around Chain O:

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

**Electron density around Chain R:**

$2mF_o-DF_c$ (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
7	NAG	A	1003	14/15	0.93	0.07	76,96,106,107	0
7	NAG	A	1006	14/15	0.94	0.08	75,102,118,120	0
10	EDO	B	1006	4/4	0.94	0.10	70,76,78,79	0
7	NAG	D	1002	14/15	0.95	0.06	70,95,104,106	0
7	NAG	C	1002	14/15	0.96	0.06	80,98,101,101	0
7	NAG	A	1004	14/15	0.96	0.06	79,95,110,113	0
7	NAG	D	1003	14/15	0.96	0.06	62,88,94,101	0
7	NAG	D	1005	14/15	0.96	0.06	80,95,101,103	0
10	EDO	A	1010	4/4	0.96	0.11	47,62,70,70	0
7	NAG	B	1004	14/15	0.96	0.05	76,90,98,98	0
7	NAG	C	1005	14/15	0.97	0.05	69,88,94,98	0
7	NAG	A	1007	14/15	0.97	0.05	60,83,93,96	0
7	NAG	A	1005	14/15	0.97	0.05	39,60,86,87	0
7	NAG	D	1004	14/15	0.97	0.04	56,75,89,92	0

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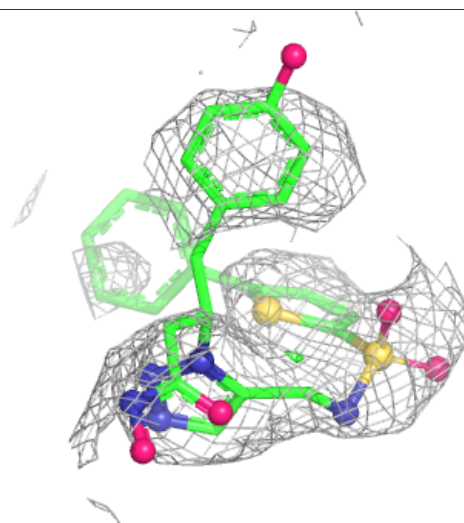
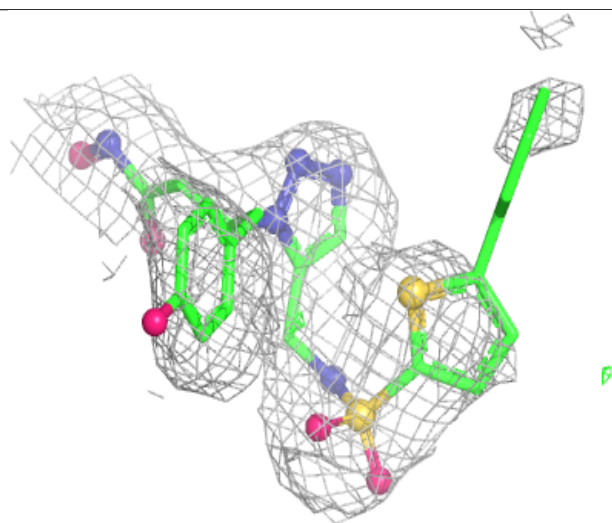
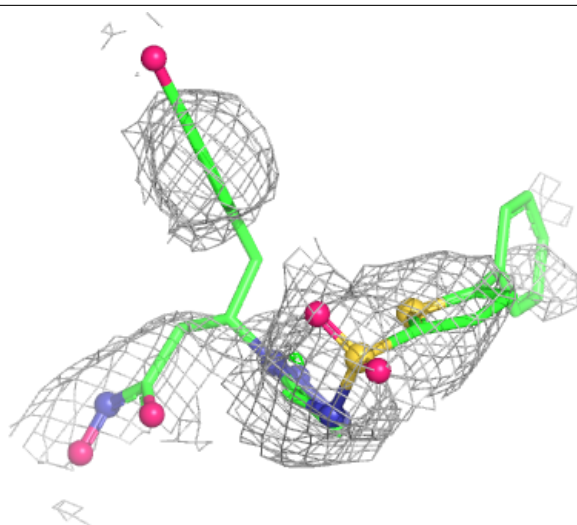
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	A	1002	14/15	0.97	0.05	78,91,97,97	0
7	NAG	C	1003	14/15	0.97	0.05	81,93,104,106	0
7	NAG	C	1004	14/15	0.97	0.04	68,89,96,96	0
11	BR	A	1016	1/1	0.97	0.06	268,268,268,268	0
11	BR	A	1017	1/1	0.97	0.12	284,284,284,284	0
7	NAG	B	1002	14/15	0.98	0.04	64,83,93,95	0
9	PGE	A	1009	10/10	0.98	0.05	42,55,62,65	0
7	NAG	B	1003	14/15	0.98	0.04	27,27,27,27	0
11	BR	C	1007	1/1	0.98	0.11	290,290,290,290	0
11	BR	C	1008	1/1	0.98	0.10	240,240,240,240	0
11	BR	D	1008	1/1	0.98	0.13	354,354,354,354	0
11	BR	A	1011	1/1	0.99	0.10	299,299,299,299	0
11	BR	A	1012	1/1	0.99	0.07	218,218,218,218	0
11	BR	A	1013	1/1	0.99	0.07	302,302,302,302	0
11	BR	A	1014	1/1	0.99	0.05	170,170,170,170	0
11	BR	A	1015	1/1	0.99	0.07	282,282,282,282	0
8	USK	D	1006	35/35	0.99	0.06	55,92,118,121	0
8	USK	A	1008	35/35	0.99	0.05	36,66,97,106	0
11	BR	A	1018	1/1	0.99	0.10	187,187,187,187	0
11	BR	B	1007	1/1	0.99	0.09	262,262,262,262	0
11	BR	B	1008	1/1	0.99	0.10	290,290,290,290	0
8	USK	B	1005	35/35	0.99	0.07	71,94,124,127	0
8	USK	C	1006	35/35	0.99	0.06	39,78,112,118	0
10	EDO	D	1007	4/4	0.99	0.03	22,41,42,46	0
6	ZN	C	1001	1/1	1.00	0.01	47,47,47,47	0
6	ZN	D	1001	1/1	1.00	0.01	41,41,41,41	0
6	ZN	A	1001	1/1	1.00	0.01	35,35,35,35	0
6	ZN	B	1001	1/1	1.00	0.02	32,32,32,32	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.

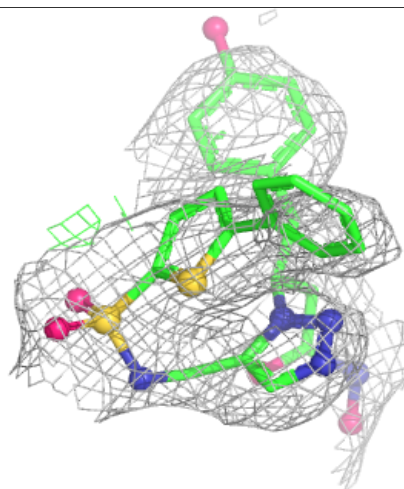
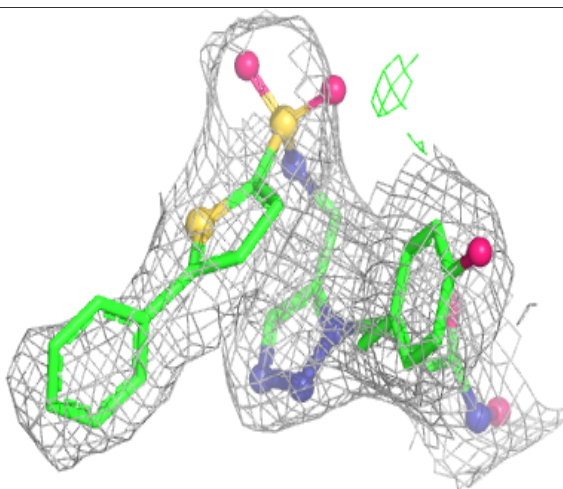
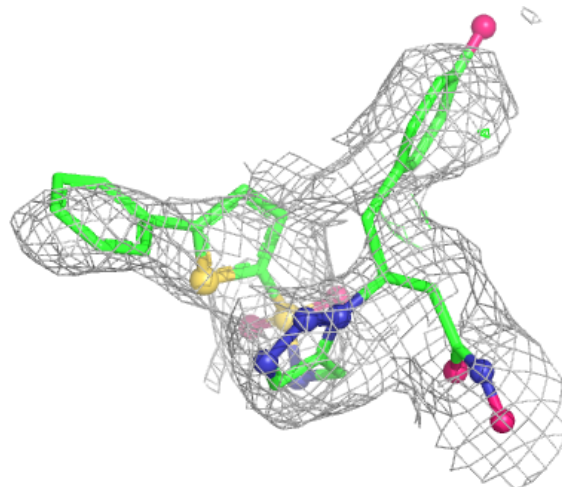
Electron density around USK D 1006:

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



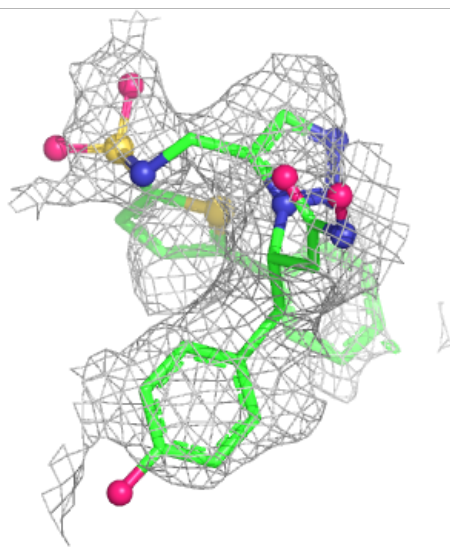
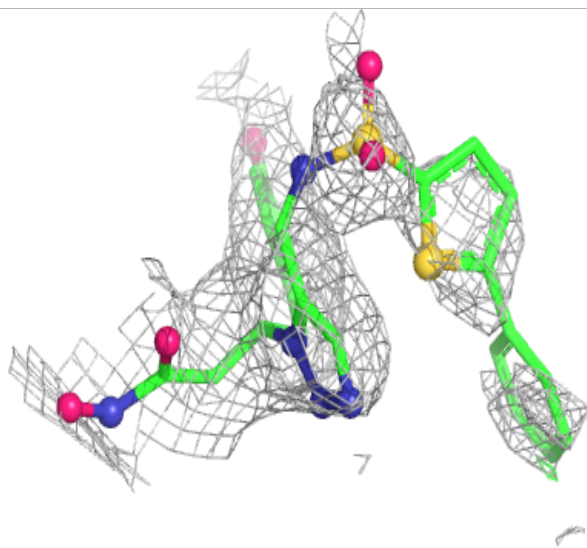
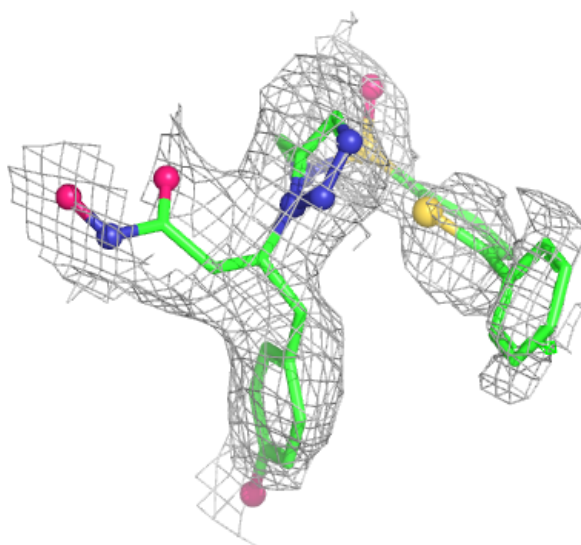
Electron density around USK A 1008:

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



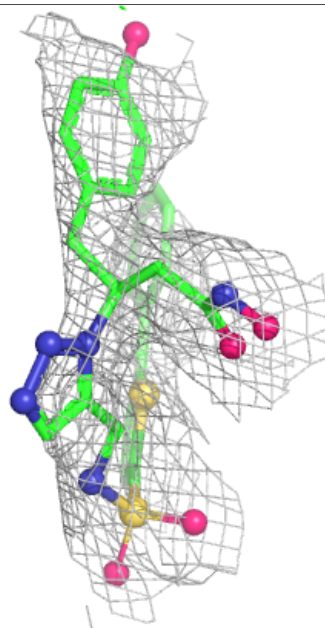
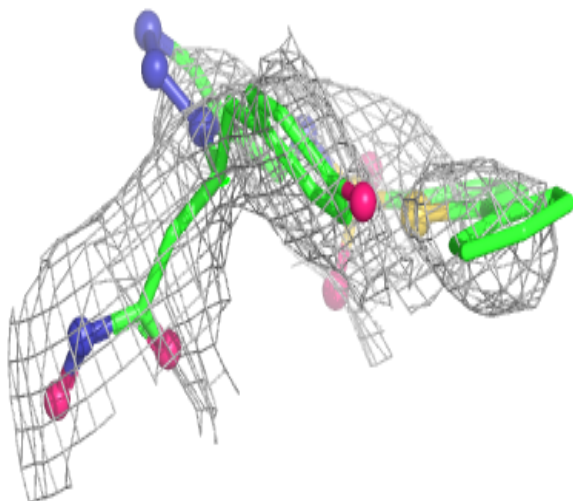
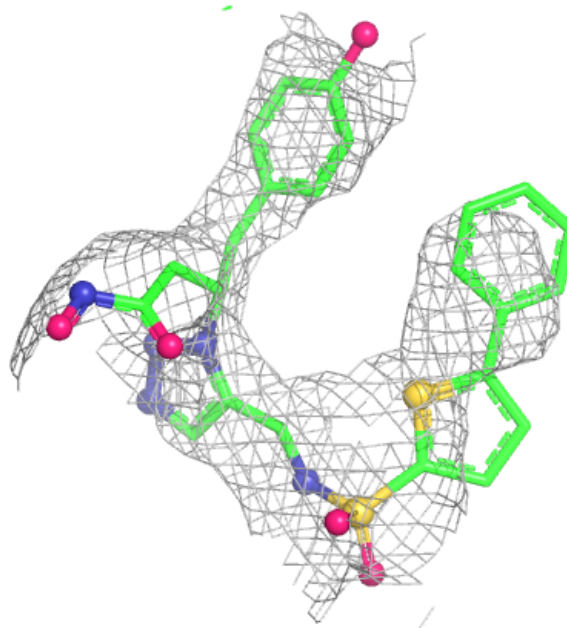
Electron density around USK B 1005:

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



Electron density around USK C 1006:

$2mF_o-DF_c$ (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.