



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 19, 2023 – 05:44 PM EDT

PDB ID : 2HRQ  
Title : Crystal structure of Human Liver Carboxylesterase 1 (hCE1) in covalent complex with the nerve agent Soman (GD)  
Authors : Fleming, C.D.; Redinbo, M.R.  
Deposited on : 2006-07-20  
Resolution : 2.70 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](mailto: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>.

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

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

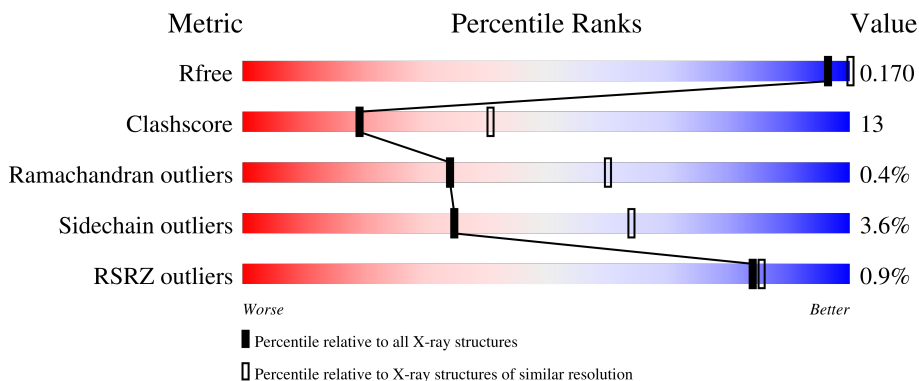
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	532	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 22%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">75%      22%      •</p>
1	B	532	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 74%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 24%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">74%      24%      •</p>
1	C	532	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 27%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">71%      27%      •</p>
1	D	532	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">73%      25%      •</p>
1	E	532	<div style="display: flex; align-items: center;"> <div style="width: 75%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 23%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">75%      23%      •</p>

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Mol	Chain	Length	Quality of chain
1	F	532	 % 75% 24%
2	G	2	100%
2	H	2	100%
2	I	2	100%
2	J	2	100%
2	K	2	100%
2	L	2	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SIA	D	482	-	-	-	X
6	SO4	F	685	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 26340 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.

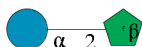
- Molecule 1 is a protein called Liver carboxylesterase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	532	4130	2662	685	763	20	0	0	0
1	B	531	4124	2659	684	761	20	0	0	0
1	C	531	4124	2659	684	761	20	0	0	0
1	D	532	4130	2662	685	763	20	0	0	0
1	E	531	4124	2659	684	761	20	0	0	0
1	F	531	4125	2659	684	762	20	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP Q9UK77
B	?	-	GLN	deletion	UNP Q9UK77
C	?	-	GLN	deletion	UNP Q9UK77
D	?	-	GLN	deletion	UNP Q9UK77
E	?	-	GLN	deletion	UNP Q9UK77
F	?	-	GLN	deletion	UNP Q9UK77

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



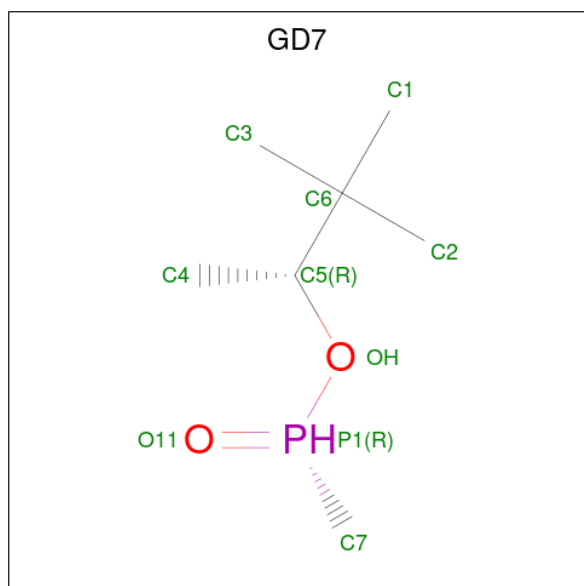
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	G	2	23	12	11	0	0	0

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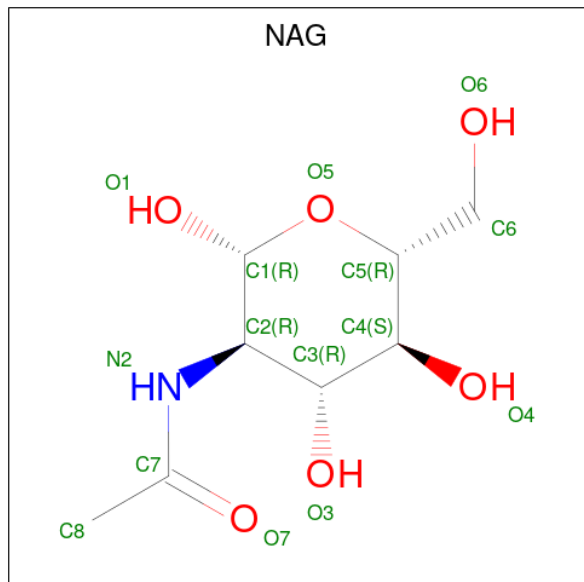
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	H	2	Total	C	O	0	0	0
			23	12	11			
2	I	2	Total	C	O	0	0	0
			23	12	11			
2	J	2	Total	C	O	0	0	0
			23	12	11			
2	K	2	Total	C	O	0	0	0
			23	12	11			
2	L	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is (1R)-1,2,2-TRIMETHYLPROPYL (R)-METHYLPHOSPHINATE (three-letter code: GD7) (formula: C<sub>7</sub>H<sub>17</sub>O<sub>2</sub>P).



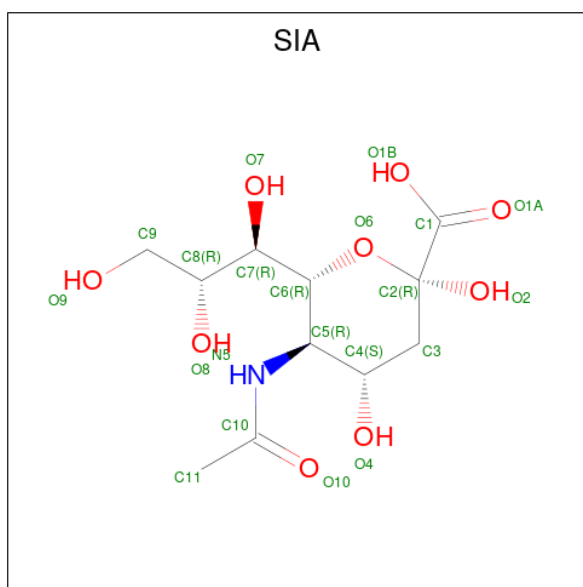
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			10	7	2	1		
3	B	1	Total	C	O	P	0	0
			10	7	2	1		
3	C	1	Total	C	O	P	0	0
			10	7	2	1		
3	D	1	Total	C	O	P	0	0
			10	7	2	1		
3	E	1	Total	C	O	P	0	0
			10	7	2	1		
3	F	1	Total	C	O	P	0	0
			10	7	2	1		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 5 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula:  $C_{11}H_{19}NO_9$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	Total	C	N	O	0	0
			21	11	1	9		
5	B	1	Total	C	N	O	0	0
			21	11	1	9		
5	C	1	Total	C	N	O	0	0
			21	11	1	9		
5	D	1	Total	C	N	O	0	0
			21	11	1	9		
5	E	1	Total	C	N	O	0	0
			21	11	1	9		
5	F	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	E	1	Total O S 5 4 1	0	0
6	F	1	Total O S 5 4 1	0	0
6	F	1	Total O S 5 4 1	0	0
6	F	1	Total O S 5 4 1	0	0

- Molecule 7 is water.

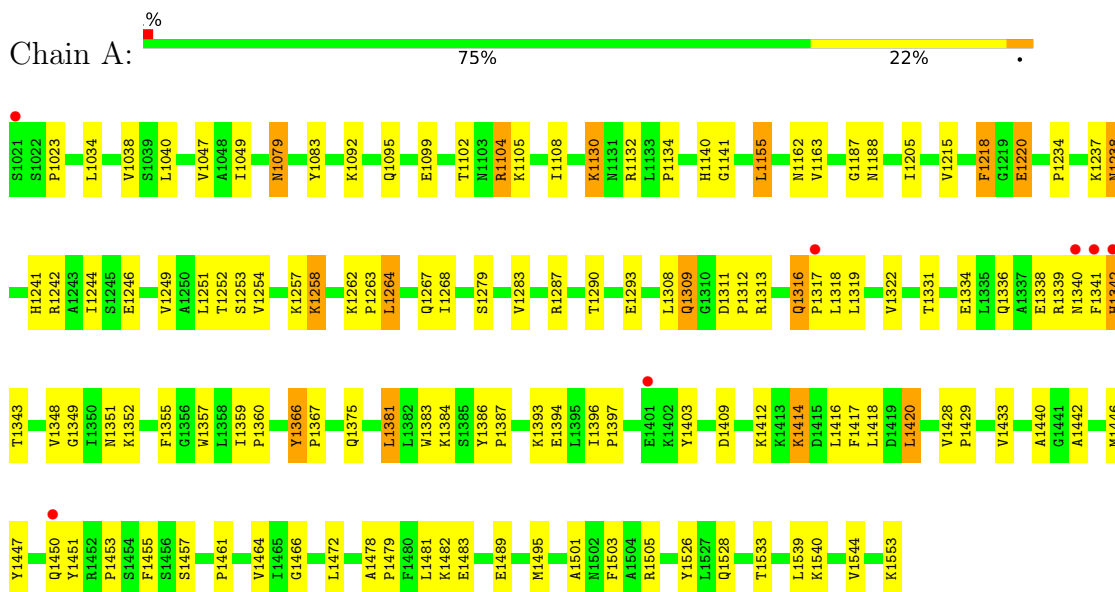


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	193	Total O 193 193	0	0
7	B	166	Total O 166 166	0	0
7	C	205	Total O 205 205	0	0
7	D	186	Total O 186 186	0	0
7	E	153	Total O 153 153	0	0
7	F	212	Total O 212 212	0	0

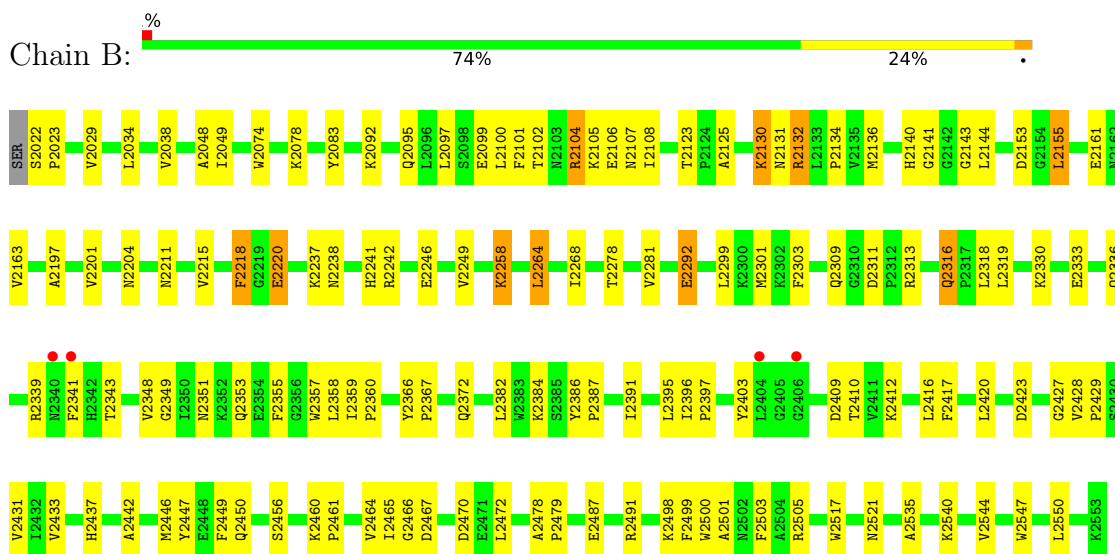
### 3 Residue-property plots

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.

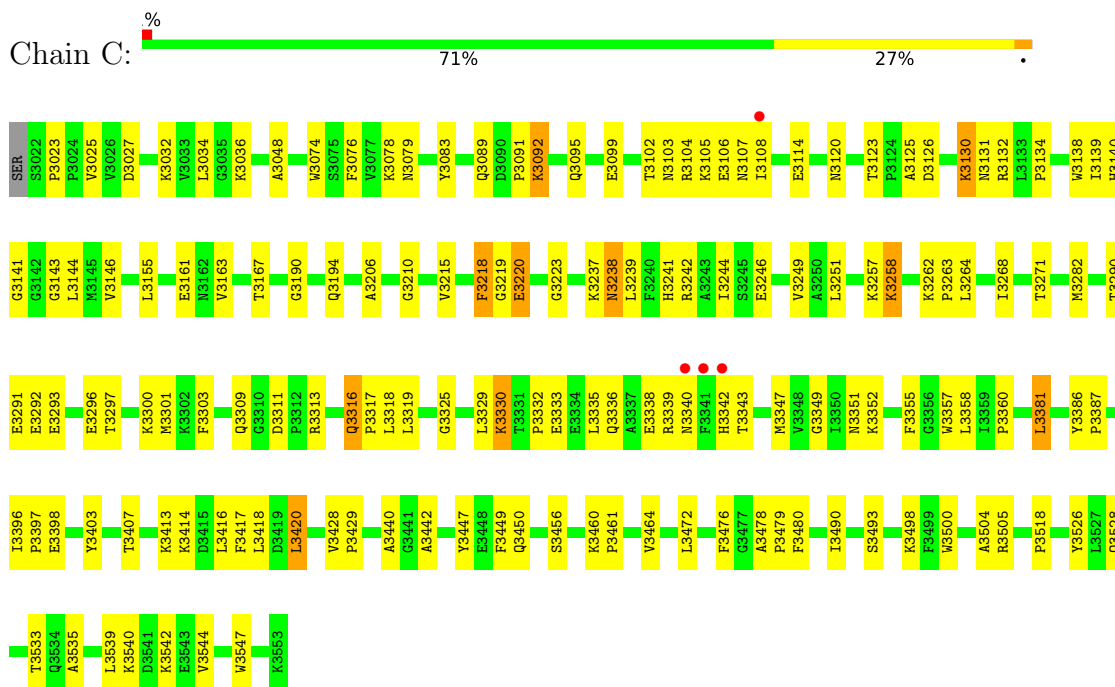
- Molecule 1: Liver carboxylesterase 1



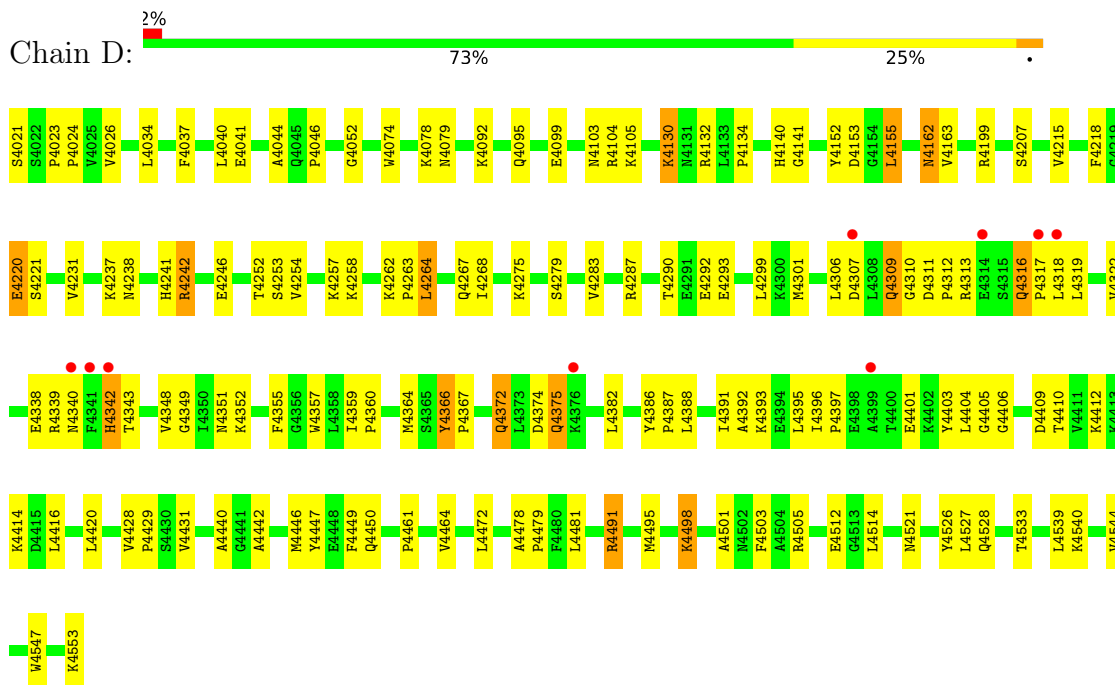
- Molecule 1: Liver carboxylesterase 1



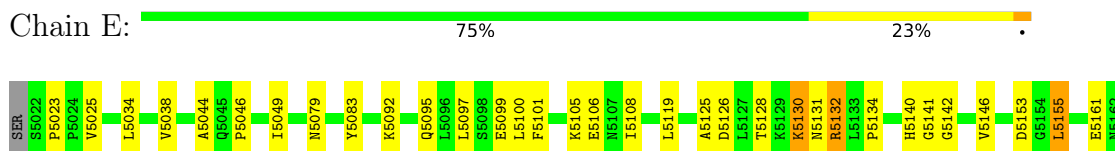
- Molecule 1: Liver carboxylesterase 1

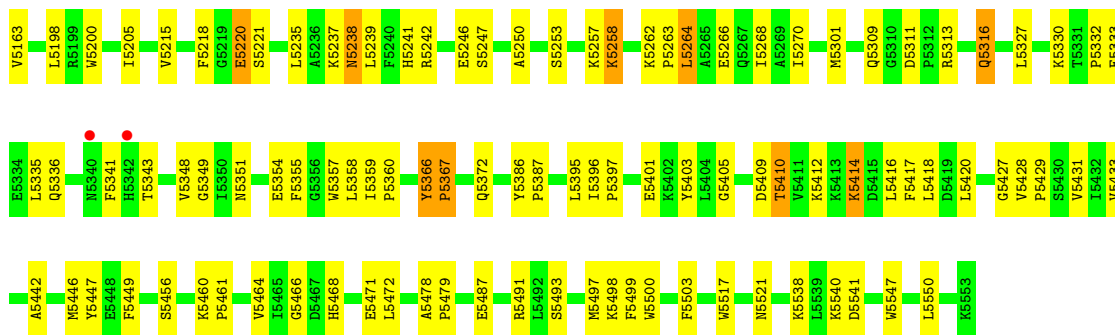


- Molecule 1: Liver carboxylesterase 1

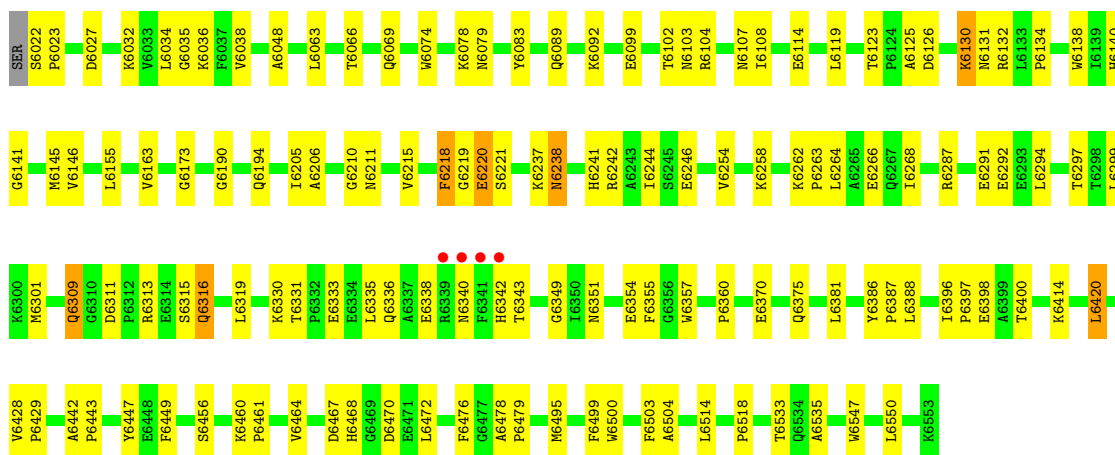
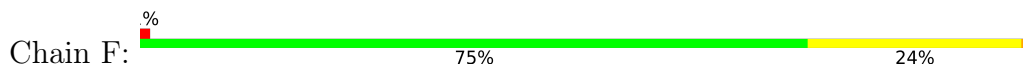


- Molecule 1: Liver carboxylesterase 1

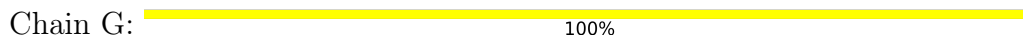




- Molecule 1: Liver carboxylesterase 1



- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



GLC1  
FRU2

- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose




GLC1  
FRU2

- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



GLC1  
FRU2

- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain J:  100%

GLC1  
FRU2

- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain K:  100%

GLC1  
FRU2

- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain L:  100%

GLC1  
FRU2

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.46Å 181.19Å 203.05Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	42.91 – 2.70 42.90 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.5 (42.91-2.70) 99.8 (42.90-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.79 (at 2.69Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.170 , 0.225 0.171 , 0.170	Depositor DCC
$R_{free}$ test set	5468 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.9	Xtrriage
Anisotropy	0.287	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 23.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.457 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	26340	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, SIA, FRU, SO4, NAG, GD7

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	0.36	1/4236 (0.0%)	0.59	1/5754 (0.0%)
1	B	0.35	1/4230 (0.0%)	0.58	1/5746 (0.0%)
1	C	0.38	1/4230 (0.0%)	0.61	1/5746 (0.0%)
1	D	0.36	1/4236 (0.0%)	0.59	1/5754 (0.0%)
1	E	0.35	1/4230 (0.0%)	0.58	1/5746 (0.0%)
1	F	0.37	1/4231 (0.0%)	0.61	1/5746 (0.0%)
All	All	0.36	6/25393 (0.0%)	0.59	6/34492 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	3092	LYS	CE-NZ	-6.21	1.33	1.49
1	F	6092	LYS	CE-NZ	-6.18	1.33	1.49
1	B	2092	LYS	CE-NZ	-6.13	1.33	1.49
1	E	5092	LYS	CE-NZ	-6.09	1.33	1.49
1	A	1092	LYS	CE-NZ	-6.08	1.33	1.49
1	D	4092	LYS	CE-NZ	-6.03	1.33	1.49

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1092	LYS	CD-CE-NZ	5.58	124.52	111.70
1	D	4092	LYS	CD-CE-NZ	5.56	124.48	111.70
1	C	3092	LYS	CD-CE-NZ	5.55	124.46	111.70
1	F	6092	LYS	CD-CE-NZ	5.51	124.38	111.70
1	E	5092	LYS	CD-CE-NZ	5.35	124.00	111.70
1	B	2092	LYS	CD-CE-NZ	5.27	123.83	111.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4130	0	4129	106	0
1	B	4124	0	4125	102	0
1	C	4124	0	4125	113	0
1	D	4130	0	4129	109	0
1	E	4124	0	4125	98	0
1	F	4125	0	4124	101	0
2	G	23	0	21	0	0
2	H	23	0	21	0	0
2	I	23	0	21	0	0
2	J	23	0	21	0	0
2	K	23	0	21	0	0
2	L	23	0	21	0	0
3	A	10	0	16	0	0
3	B	10	0	16	0	0
3	C	10	0	16	0	0
3	D	10	0	16	0	0
3	E	10	0	16	2	0
3	F	10	0	16	0	0
4	A	14	0	13	5	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
4	E	14	0	13	1	0
4	F	14	0	13	2	0
5	A	21	0	18	6	0
5	B	21	0	18	5	0
5	C	21	0	18	5	0
5	D	21	0	18	2	0
5	E	21	0	18	6	0
5	F	21	0	18	4	0
6	A	10	0	0	0	0
6	B	10	0	0	0	0
6	C	10	0	0	1	0
6	D	10	0	0	0	0
6	E	5	0	0	0	0
6	F	15	0	0	0	0
7	A	193	0	0	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	166	0	0	11	0
7	C	205	0	0	8	0
7	D	186	0	0	11	0
7	E	153	0	0	6	0
7	F	212	0	0	9	0
All	All	26340	0	25165	648	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 13.

All (648) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:179:NAG:H82	7:A:8924:HOH:O	1.48	1.12
1:C:3343:THR:HB	1:C:3442:ALA:HB2	1.23	1.11
1:F:6343:THR:HB	1:F:6442:ALA:HB2	1.14	1.10
1:D:4491:ARG:HH11	1:D:4491:ARG:HB2	1.17	1.08
1:A:1079:ASN:H	5:A:182:SIA:H112	1.23	1.00
4:A:179:NAG:C8	7:A:8924:HOH:O	2.04	0.99
1:D:4215:VAL:H	1:D:4241:HIS:HD2	1.09	0.98
1:B:2220:GLU:HG2	1:B:2472:LEU:HD21	1.46	0.97
1:C:3215:VAL:H	1:C:3241:HIS:HD2	1.10	0.96
1:A:1215:VAL:H	1:A:1241:HIS:HD2	1.10	0.96
1:D:4307:ASP:HB3	7:D:8090:HOH:O	1.68	0.92
1:F:6215:VAL:H	1:F:6241:HIS:HD2	1.19	0.91
1:D:4352:LYS:HD3	1:D:4450:GLN:HE21	1.36	0.89
1:A:1352:LYS:HD3	1:A:1450:GLN:HE21	1.37	0.87
1:C:3237:LYS:O	1:C:3238:ASN:HB2	1.75	0.85
1:D:4290:THR:OG1	1:D:4293:GLU:HG3	1.77	0.85
1:E:5215:VAL:H	1:E:5241:HIS:HD2	1.23	0.85
1:E:5220:GLU:HG2	1:E:5472:LEU:HD21	1.58	0.83
1:E:5395:LEU:HB3	1:E:5550:LEU:HD11	1.60	0.81
1:D:4242:ARG:HG2	1:D:4242:ARG:HH11	1.46	0.81
1:D:4343:THR:HB	1:D:4442:ALA:HB2	1.62	0.81
1:D:4279:SER:H	5:F:682:SIA:H111	1.45	0.81
1:F:6242:ARG:HG2	1:F:6242:ARG:HH11	1.44	0.80
1:E:5343:THR:HB	1:E:5442:ALA:HB2	1.64	0.79
4:A:179:NAG:N2	7:A:8924:HOH:O	2.14	0.79
1:D:4396:ILE:HB	1:D:4397:PRO:HD3	1.63	0.79
1:C:3290:THR:HB	1:C:3292:GLU:OE1	1.82	0.79
1:C:3125:ALA:HB1	1:C:3131:ASN:HD22	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2125:ALA:HB1	1:B:2131:ASN:HD22	1.50	0.77
1:A:1095:GLN:O	1:A:1099:GLU:HG3	1.85	0.76
1:F:6398:GLU:HG3	7:F:8804:HOH:O	1.85	0.76
1:D:4023:PRO:HB2	1:D:4034:LEU:HD21	1.67	0.76
1:A:1396:ILE:HB	1:A:1397:PRO:HD3	1.67	0.76
1:B:2215:VAL:H	1:B:2241:HIS:HD2	1.32	0.76
1:A:1268:ILE:HD11	1:A:1319:LEU:HD21	1.68	0.76
1:D:4095:GLN:O	1:D:4099:GLU:HG3	1.87	0.75
1:A:1343:THR:HB	1:A:1442:ALA:HB2	1.69	0.75
1:C:3242:ARG:HG2	1:C:3242:ARG:HH11	1.51	0.74
1:D:4215:VAL:H	1:D:4241:HIS:CD2	2.00	0.74
1:D:4242:ARG:HH11	1:D:4242:ARG:CG	2.00	0.74
1:D:4491:ARG:HH11	1:D:4491:ARG:CB	1.97	0.74
1:E:5134:PRO:HG2	1:E:5163:VAL:HG12	1.67	0.74
1:D:4428:VAL:HG13	1:D:4544:VAL:HG22	1.67	0.74
1:A:1215:VAL:H	1:A:1241:HIS:CD2	2.01	0.74
1:C:3083:TYR:CE2	1:C:3108:ILE:HD13	2.23	0.74
1:D:4130:LYS:HD2	1:D:4130:LYS:O	1.86	0.74
1:F:6215:VAL:H	1:F:6241:HIS:CD2	2.05	0.73
1:B:2501:ALA:HB1	1:B:2505:ARG:HH12	1.53	0.73
1:F:6130:LYS:HD2	1:F:6130:LYS:O	1.89	0.73
1:C:3099:GLU:HA	1:C:3107:ASN:HD22	1.54	0.73
1:E:5355:PHE:CE1	1:E:5360:PRO:HG3	2.24	0.73
5:B:282:SIA:H7	7:B:8086:HOH:O	1.89	0.73
1:D:4403:TYR:O	1:D:4416:LEU:HD13	1.89	0.72
1:E:5428:VAL:HB	1:E:5429:PRO:HD3	1.70	0.72
1:A:1023:PRO:HB2	1:A:1034:LEU:HD21	1.71	0.72
1:B:2428:VAL:HB	1:B:2429:PRO:HD3	1.70	0.72
1:C:3134:PRO:HG2	1:C:3163:VAL:HG12	1.70	0.72
1:F:6220:GLU:HG2	1:F:6472:LEU:HD21	1.72	0.72
1:A:1237:LYS:O	1:A:1238:ASN:HB2	1.90	0.71
1:F:6238:ASN:HB2	7:F:8536:HOH:O	1.91	0.71
1:A:1130:LYS:HD2	1:A:1130:LYS:O	1.90	0.71
1:C:3215:VAL:H	1:C:3241:HIS:CD2	2.00	0.71
1:E:5409:ASP:HB3	1:E:5412:LYS:HB2	1.71	0.71
1:E:5242:ARG:HG2	1:E:5242:ARG:HH11	1.55	0.70
1:B:2343:THR:HA	7:B:8097:HOH:O	1.91	0.70
1:C:3027:ASP:OD1	1:C:3032:LYS:HG2	1.92	0.70
5:D:482:SIA:H91	7:D:8005:HOH:O	1.92	0.70
1:D:4134:PRO:HG2	1:D:4163:VAL:HG12	1.73	0.69
1:C:3340:ASN:HB3	7:C:8044:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1290:THR:OG1	1:A:1293:GLU:HG3	1.93	0.69
1:E:5100:LEU:HD13	1:E:5358:LEU:CD1	2.23	0.69
1:E:5491:ARG:HD2	7:E:8313:HOH:O	1.92	0.69
1:D:4237:LYS:O	1:D:4238:ASN:HB2	1.92	0.69
1:B:2023:PRO:HB2	1:B:2034:LEU:HD21	1.75	0.69
1:C:3355:PHE:CE1	1:C:3360:PRO:HG3	2.29	0.68
1:A:1262:LYS:HB3	1:A:1263:PRO:HD3	1.75	0.68
1:A:1308:LEU:HB2	7:A:8294:HOH:O	1.94	0.68
1:D:4263:PRO:O	1:D:4267:GLN:HG3	1.93	0.68
1:A:1241:HIS:O	1:A:1242:ARG:HG3	1.93	0.68
1:A:1316:GLN:HG3	7:A:8045:HOH:O	1.92	0.67
5:E:582:SIA:H6	5:E:582:SIA:H113	1.76	0.67
1:F:6355:PHE:CE1	1:F:6360:PRO:HG3	2.30	0.67
1:B:2134:PRO:HG2	1:B:2163:VAL:HG12	1.76	0.67
1:D:4292:GLU:HG3	7:D:8756:HOH:O	1.95	0.67
1:B:2409:ASP:HB3	1:B:2412:LYS:HB2	1.75	0.66
1:F:6083:TYR:CE2	1:F:6108:ILE:HD13	2.29	0.66
1:D:4262:LYS:HE3	1:D:4279:SER:OG	1.96	0.66
1:A:1242:ARG:HG2	1:A:1242:ARG:HH11	1.61	0.66
1:B:2125:ALA:HB1	1:B:2131:ASN:ND2	2.10	0.66
1:D:4262:LYS:HB3	1:D:4263:PRO:HD3	1.78	0.66
1:A:1220:GLU:HG2	1:A:1472:LEU:HD21	1.77	0.65
1:B:2083:TYR:CE2	1:B:2108:ILE:HD13	2.31	0.65
1:E:5105:LYS:HG3	1:E:5106:GLU:H	1.60	0.65
1:B:2100:LEU:HD13	1:B:2358:LEU:CD1	2.26	0.65
1:A:1501:ALA:O	1:A:1505:ARG:HG2	1.97	0.65
1:B:2355:PHE:CE1	1:B:2360:PRO:HG3	2.31	0.65
1:A:1339:ARG:HD3	1:A:1440:ALA:HA	1.79	0.64
1:D:4501:ALA:O	1:D:4505:ARG:HG2	1.96	0.64
1:A:1403:TYR:O	1:A:1416:LEU:HD13	1.97	0.64
1:B:2100:LEU:HD13	1:B:2358:LEU:HD11	1.79	0.64
1:C:3130:LYS:HD2	1:C:3130:LYS:O	1.97	0.64
1:B:2501:ALA:HB1	1:B:2505:ARG:NH1	2.13	0.64
1:D:4339:ARG:HD3	1:D:4440:ALA:HA	1.80	0.64
1:D:4355:PHE:CE1	1:D:4360:PRO:HG3	2.32	0.64
1:A:1079:ASN:N	5:A:182:SIA:H112	2.06	0.63
1:F:6495:MET:HE3	1:F:6533:THR:HG21	1.79	0.63
1:B:2105:LYS:HG3	7:B:8556:HOH:O	1.98	0.63
1:A:1352:LYS:CD	1:A:1450:GLN:HE21	2.09	0.63
1:A:1242:ARG:HH11	1:A:1242:ARG:CG	2.12	0.63
1:D:4409:ASP:HB3	1:D:4412:LYS:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1553:LYS:HB2	1:A:1553:LYS:NZ	2.14	0.63
1:D:4241:HIS:O	1:D:4242:ARG:HG3	1.98	0.62
1:C:3290:THR:HA	6:C:184:SO4:O2	1.99	0.62
1:F:6258:LYS:NZ	1:F:6333:GLU:OE2	2.32	0.62
1:C:3258:LYS:HD2	1:C:3258:LYS:O	1.99	0.62
1:F:6237:LYS:HD2	1:F:6342:HIS:CD2	2.34	0.62
1:F:6357:TRP:O	1:F:6360:PRO:HD2	2.00	0.62
1:D:4231:VAL:HG13	7:D:8593:HOH:O	1.99	0.61
1:E:5403:TYR:O	1:E:5416:LEU:HD13	2.00	0.61
1:B:2242:ARG:HG2	1:B:2242:ARG:HH11	1.66	0.61
5:E:582:SIA:H113	7:F:8178:HOH:O	2.00	0.61
1:E:5333:GLU:N	1:E:5333:GLU:OE1	2.29	0.61
1:F:6351:ASN:ND2	1:F:6449:PHE:HB3	2.15	0.61
1:A:1352:LYS:HB2	1:A:1450:GLN:HG2	1.82	0.61
1:B:2349:GLY:HA3	1:B:2447:TYR:CE1	2.35	0.61
1:F:6268:ILE:HD11	1:F:6319:LEU:HD21	1.83	0.61
4:A:179:NAG:C7	7:A:8924:HOH:O	2.36	0.60
1:A:1409:ASP:HB3	1:A:1412:LYS:HB2	1.84	0.60
1:D:4372:GLN:HG2	1:D:4410:THR:HB	1.84	0.60
1:E:5083:TYR:CE2	1:E:5108:ILE:HD13	2.37	0.60
1:F:6338:GLU:HG2	1:F:6340:ASN:HD22	1.67	0.60
1:C:3311:ASP:OD1	1:C:3313:ARG:HB2	2.01	0.60
1:A:1241:HIS:C	1:A:1242:ARG:HG3	2.23	0.59
1:B:2431:VAL:HG21	1:B:2540:LYS:HB2	1.84	0.59
1:C:3237:LYS:O	1:C:3238:ASN:CB	2.49	0.59
1:E:5130:LYS:NZ	1:E:5130:LYS:HB3	2.17	0.59
1:D:4220:GLU:HG2	1:D:4472:LEU:HD21	1.84	0.59
1:D:4241:HIS:C	1:D:4242:ARG:HG3	2.23	0.59
1:A:1251:LEU:HB2	1:A:1429:PRO:HB3	1.84	0.59
1:C:3220:GLU:HG2	1:C:3472:LEU:HD21	1.84	0.59
1:E:5396:ILE:HB	1:E:5397:PRO:HD3	1.85	0.59
1:F:6311:ASP:OD1	1:F:6313:ARG:HB2	2.02	0.59
1:A:1262:LYS:HE3	1:A:1279:SER:OG	2.03	0.59
1:C:3126:ASP:H	1:C:3131:ASN:ND2	2.00	0.59
1:D:4140:HIS:HD2	1:D:4141:GLY:O	1.85	0.59
1:C:3351:ASN:ND2	1:C:3449:PHE:HB3	2.16	0.59
5:E:582:SIA:H7	7:E:8014:HOH:O	2.03	0.59
1:F:6134:PRO:HG2	1:F:6163:VAL:HG12	1.85	0.59
1:A:1079:ASN:H	5:A:182:SIA:C11	2.09	0.58
1:C:3257:LYS:NZ	1:C:3316:GLN:HG3	2.18	0.58
1:F:6103:ASN:ND2	1:F:6476:PHE:HB3	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2403:TYR:CD1	1:B:2420:LEU:HD13	2.38	0.58
5:C:382:SIA:H91	5:C:382:SIA:H5	1.86	0.58
1:A:1140:HIS:HD2	1:A:1141:GLY:O	1.87	0.58
1:A:1258:LYS:HD2	7:A:8961:HOH:O	2.03	0.58
5:B:282:SIA:C11	1:C:3262:LYS:NZ	2.66	0.58
1:D:4382:LEU:HD23	1:D:4396:ILE:HG23	1.85	0.58
1:E:5132:ARG:HE	1:E:5132:ARG:HA	1.67	0.58
1:E:5355:PHE:CD1	1:E:5360:PRO:HG3	2.38	0.58
1:F:6125:ALA:HB1	1:F:6131:ASN:HD22	1.68	0.58
1:C:3333:GLU:N	1:C:3333:GLU:OE1	2.33	0.58
1:D:4215:VAL:N	1:D:4241:HIS:HD2	1.92	0.58
1:C:3357:TRP:O	1:C:3360:PRO:HD2	2.03	0.57
1:D:4242:ARG:CG	1:D:4242:ARG:NH1	2.64	0.57
1:F:6396:ILE:HB	1:F:6397:PRO:HD3	1.86	0.57
1:B:2396:ILE:HB	1:B:2397:PRO:HD3	1.85	0.57
1:B:2456:SER:HB3	1:B:2460:LYS:HD3	1.85	0.57
1:E:5023:PRO:HB2	1:E:5034:LEU:HD21	1.86	0.57
1:C:3398:GLU:HB3	7:C:8219:HOH:O	2.05	0.57
1:B:2237:LYS:O	1:B:2238:ASN:HB2	2.04	0.56
1:B:2372:GLN:HB2	1:B:2410:THR:HB	1.87	0.56
1:C:3338:GLU:HB3	7:C:8044:HOH:O	2.04	0.56
1:E:5079:ASN:O	5:E:582:SIA:O2	2.22	0.56
1:B:2355:PHE:CD1	1:B:2360:PRO:HG3	2.40	0.56
1:C:3023:PRO:CB	1:C:3034:LEU:HD21	2.35	0.56
1:D:4382:LEU:HD11	1:D:4391:ILE:HD12	1.88	0.56
1:E:5237:LYS:C	7:E:8004:HOH:O	2.43	0.56
1:E:5237:LYS:O	1:E:5237:LYS:HG3	2.05	0.56
1:F:6375:GLN:HE22	1:F:6400:THR:HG22	1.71	0.56
1:C:3114:GLU:HG3	1:C:3291:GLU:HG3	1.88	0.56
1:E:5097:LEU:HD11	1:E:5101:PHE:CE2	2.41	0.56
1:B:2333:GLU:N	1:B:2333:GLU:OE1	2.38	0.56
1:E:5348:VAL:O	1:E:5446:MET:HA	2.06	0.55
1:C:3237:LYS:HG3	1:C:3342:HIS:HB2	1.89	0.55
1:A:1023:PRO:CB	1:A:1034:LEU:HD21	2.36	0.55
1:B:2095:GLN:O	1:B:2099:GLU:HG3	2.07	0.55
1:F:6420:LEU:HD13	1:F:6547:TRP:HZ2	1.71	0.55
1:E:5130:LYS:HB3	1:E:5130:LYS:HZ3	1.71	0.55
1:F:6386:TYR:N	1:F:6387:PRO:HD2	2.22	0.55
1:A:1134:PRO:HG2	1:A:1163:VAL:HG12	1.88	0.55
1:C:3542:LYS:HG2	7:C:9086:HOH:O	2.07	0.55
1:D:4268:ILE:HD11	1:D:4319:LEU:HD21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5351:ASN:HB3	1:E:5466:GLY:O	2.06	0.55
1:E:5456:SER:HB3	1:E:5460:LYS:HD3	1.87	0.55
1:F:6420:LEU:HD13	1:F:6547:TRP:CZ2	2.42	0.54
1:E:5351:ASN:ND2	1:E:5449:PHE:HB3	2.23	0.54
1:C:3023:PRO:HB2	1:C:3034:LEU:HD21	1.89	0.54
1:D:4257:LYS:HB2	1:D:4322:VAL:HG12	1.88	0.54
1:D:4264:LEU:HG	1:D:4316:GLN:HG2	1.88	0.54
1:F:6242:ARG:HG2	1:F:6242:ARG:NH1	2.18	0.54
1:C:3297:THR:O	1:C:3301:MET:HG2	2.07	0.54
1:E:5257:LYS:HZ1	1:E:5316:GLN:HG3	1.73	0.54
1:C:3292:GLU:CD	1:C:3292:GLU:H	2.11	0.54
1:C:3407:THR:O	1:C:3413:LYS:HE2	2.07	0.54
1:F:6023:PRO:HB2	1:F:6034:LEU:HD21	1.89	0.54
1:D:4290:THR:HG1	1:D:4293:GLU:HG3	1.70	0.54
1:D:4348:VAL:O	1:D:4446:MET:HA	2.08	0.54
1:A:1386:TYR:N	1:A:1387:PRO:HD2	2.23	0.54
1:D:4372:GLN:CG	1:D:4410:THR:HB	2.37	0.54
1:E:5420:LEU:CD1	1:E:5547:TRP:HZ2	2.20	0.54
1:C:3386:TYR:N	1:C:3387:PRO:HD2	2.23	0.53
1:A:1083:TYR:CE2	1:A:1108:ILE:HD13	2.43	0.53
1:F:6237:LYS:O	1:F:6237:LYS:HG3	2.07	0.53
1:A:1246:GLU:HG2	1:A:1447:TYR:OH	2.09	0.53
1:E:5403:TYR:CD1	1:E:5420:LEU:HD13	2.43	0.53
1:A:1359:ILE:HB	1:A:1360:PRO:HD3	1.89	0.53
1:B:2258:LYS:HD2	1:B:2258:LYS:O	2.08	0.53
1:C:3099:GLU:HA	1:C:3107:ASN:ND2	2.22	0.53
1:D:4339:ARG:CD	1:D:4440:ALA:HA	2.38	0.53
1:A:1257:LYS:HB2	1:A:1322:VAL:HG12	1.89	0.53
1:B:2349:GLY:HA3	1:B:2447:TYR:CZ	2.44	0.53
1:E:5359:ILE:HB	1:E:5360:PRO:HD3	1.90	0.53
1:B:2403:TYR:O	1:B:2416:LEU:HD13	2.09	0.52
1:A:1451:TYR:CE2	1:A:1489:GLU:HG3	2.44	0.52
1:F:6297:THR:O	1:F:6301:MET:HG2	2.08	0.52
1:A:1262:LYS:HZ3	5:C:382:SIA:H113	1.75	0.52
1:C:3048:ALA:HB3	1:C:3123:THR:HG23	1.90	0.52
1:F:6354:GLU:O	1:F:6468:HIS:HB2	2.09	0.52
1:F:6370:GLU:HB2	7:F:8655:HOH:O	2.09	0.52
1:D:4428:VAL:HB	1:D:4429:PRO:HD3	1.91	0.52
1:F:6099:GLU:HA	1:F:6107:ASN:ND2	2.24	0.52
1:E:5025:VAL:HG22	1:E:5034:LEU:HD23	1.91	0.52
1:E:5429:PRO:O	1:E:5433:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6102:THR:OG1	1:F:6104:ARG:HG2	2.09	0.52
1:A:1342:HIS:O	1:A:1342:HIS:CD2	2.63	0.52
1:E:5401:GLU:OE2	1:E:5405:GLY:HA3	2.10	0.52
1:A:1348:VAL:O	1:A:1446:MET:HA	2.10	0.51
1:D:4461:PRO:HG2	1:D:4464:VAL:CG2	2.41	0.51
1:A:1451:TYR:HE2	1:A:1489:GLU:HG3	1.74	0.51
1:D:4521:ASN:HB2	7:D:8625:HOH:O	2.10	0.51
1:E:5140:HIS:HD2	1:E:5141:GLY:O	1.93	0.51
1:C:3105:LYS:HG3	1:C:3106:GLU:H	1.74	0.51
1:C:3242:ARG:HG2	1:C:3242:ARG:NH1	2.23	0.51
1:F:6428:VAL:HB	1:F:6429:PRO:HD3	1.91	0.51
1:E:5349:GLY:HA3	1:E:5447:TYR:CE1	2.45	0.51
1:F:6478:ALA:N	1:F:6479:PRO:CD	2.73	0.51
1:B:2105:LYS:HG3	1:B:2106:GLU:H	1.74	0.51
1:B:2341:PHE:HA	7:B:8642:HOH:O	2.10	0.51
1:C:3478:ALA:N	1:C:3479:PRO:CD	2.74	0.51
1:E:5386:TYR:N	1:E:5387:PRO:HD2	2.25	0.51
1:B:2427:GLY:O	1:B:2431:VAL:HG23	2.09	0.51
1:D:4351:ASN:ND2	1:D:4449:PHE:HB3	2.26	0.51
1:B:2351:ASN:HB3	1:B:2466:GLY:O	2.10	0.51
1:F:6126:ASP:H	1:F:6131:ASN:ND2	2.08	0.51
1:B:2143:GLY:O	1:B:2318:LEU:HD22	2.11	0.51
1:B:2450:GLN:HB2	7:B:8218:HOH:O	2.10	0.51
1:C:3262:LYS:HE2	1:C:3282:MET:HE1	1.93	0.51
1:E:5487:GLU:O	1:E:5491:ARG:HG3	2.10	0.51
1:B:2461:PRO:HG2	1:B:2464:VAL:CG2	2.41	0.51
1:C:3428:VAL:HB	1:C:3429:PRO:HD3	1.92	0.51
1:D:4349:GLY:HA3	1:D:4447:TYR:CE1	2.46	0.51
1:F:6336:GLN:C	1:F:6338:GLU:H	2.15	0.51
1:C:3420:LEU:HD13	1:C:3547:TRP:HZ2	1.75	0.50
1:E:5431:VAL:HG21	1:E:5540:LYS:HB2	1.93	0.50
1:F:6330:LYS:HG3	1:F:6335:LEU:CD2	2.42	0.50
1:C:3268:ILE:HD11	1:C:3319:LEU:HD21	1.94	0.50
1:B:2386:TYR:N	1:B:2387:PRO:HD2	2.26	0.50
5:C:382:SIA:O7	7:C:8364:HOH:O	2.18	0.50
1:E:5153:ASP:OD2	1:E:5155:LEU:HB2	2.11	0.50
1:E:5257:LYS:NZ	1:E:5316:GLN:HG3	2.26	0.50
4:F:679:NAG:O6	5:F:682:SIA:O1A	2.23	0.50
1:B:2140:HIS:HD2	1:B:2141:GLY:O	1.94	0.50
1:B:2395:LEU:HB3	1:B:2550:LEU:HD11	1.94	0.50
1:F:6262:LYS:O	1:F:6266:GLU:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2099:GLU:HA	1:B:2107:ASN:ND2	2.27	0.50
1:B:2461:PRO:HG2	1:B:2464:VAL:HG23	1.93	0.50
1:B:2391:ILE:HA	7:B:8452:HOH:O	2.10	0.50
1:E:5095:GLN:O	1:E:5099:GLU:HG3	2.12	0.50
1:E:5336:GLN:HE22	1:E:5433:VAL:HA	1.76	0.50
1:A:1262:LYS:NZ	5:C:382:SIA:H113	2.26	0.50
1:C:3132:ARG:NE	7:C:8507:HOH:O	2.43	0.50
1:F:6036:LYS:HD3	7:F:8425:HOH:O	2.10	0.50
1:A:1338:GLU:C	1:A:1340:ASN:N	2.65	0.50
1:C:3190:GLY:O	1:C:3194:GLN:HG3	2.12	0.50
1:C:3242:ARG:NE	1:C:3504:ALA:O	2.45	0.50
1:E:5237:LYS:O	1:E:5238:ASN:CB	2.58	0.50
1:A:1242:ARG:CG	1:A:1242:ARG:NH1	2.72	0.49
1:A:1264:LEU:HG	1:A:1316:GLN:HG2	1.93	0.49
1:B:2521:ASN:HB2	7:B:8215:HOH:O	2.11	0.49
1:C:3420:LEU:HD13	1:C:3547:TRP:CZ2	2.47	0.49
1:A:1457:SER:HA	7:A:8224:HOH:O	2.11	0.49
1:B:2097:LEU:HD11	1:B:2101:PHE:CE2	2.46	0.49
1:B:2535:ALA:N	7:B:8663:HOH:O	2.42	0.49
1:C:3140:HIS:HD2	1:C:3141:GLY:O	1.96	0.49
1:F:6022:SER:N	7:F:8665:HOH:O	2.45	0.49
1:C:3396:ILE:HB	1:C:3397:PRO:HD3	1.94	0.49
1:E:5242:ARG:HD3	1:E:5503:PHE:O	2.12	0.49
1:E:5349:GLY:HA3	1:E:5447:TYR:CZ	2.48	0.49
1:E:5478:ALA:N	1:E:5479:PRO:CD	2.76	0.49
1:F:6027:ASP:HA	1:F:6032:LYS:HA	1.94	0.49
1:B:2301:MET:HB2	1:B:2303:PHE:CE1	2.48	0.49
1:C:3239:LEU:HG	7:C:8271:HOH:O	2.13	0.49
1:C:3352:LYS:HG2	1:C:3450:GLN:HE21	1.77	0.49
1:D:4306:LEU:HD22	1:D:4366:TYR:CE1	2.48	0.49
1:B:2292:GLU:CD	1:B:2292:GLU:H	2.16	0.49
1:C:3325:GLY:HA2	1:C:3329:LEU:HD23	1.95	0.49
1:F:6099:GLU:HA	1:F:6107:ASN:HD22	1.78	0.49
1:F:6241:HIS:C	1:F:6242:ARG:HG3	2.33	0.49
1:C:3079:ASN:HB2	5:C:382:SIA:C1	2.42	0.49
1:E:5332:PRO:O	1:E:5336:GLN:HG3	2.13	0.49
1:C:3237:LYS:CG	1:C:3342:HIS:HB2	2.43	0.49
1:C:3251:LEU:HD21	1:C:3333:GLU:HG3	1.94	0.49
1:C:3355:PHE:CD1	1:C:3360:PRO:HG3	2.48	0.49
1:D:4392:ALA:HB3	1:D:4395:LEU:HG	1.93	0.49
1:F:6218:PHE:CB	1:F:6244:ILE:HB	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2336:GLN:HE22	1:B:2433:VAL:HA	1.77	0.48
1:E:5354:GLU:O	1:E:5468:HIS:HB2	2.13	0.48
1:C:3089:GLN:HB2	1:C:3146:VAL:HG12	1.94	0.48
1:D:4317:PRO:HD3	1:D:4387:PRO:HB2	1.95	0.48
1:E:5125:ALA:HB1	1:E:5131:ASN:ND2	2.28	0.48
1:B:2429:PRO:O	1:B:2433:VAL:HG23	2.13	0.48
1:B:2478:ALA:N	1:B:2479:PRO:CD	2.77	0.48
1:D:4528:GLN:O	1:D:4533:THR:HG23	2.12	0.48
1:A:1238:ASN:ND2	7:A:8687:HOH:O	2.47	0.48
1:B:2450:GLN:O	1:B:2450:GLN:HG2	2.12	0.48
1:E:5372:GLN:HB3	1:E:5410:THR:HB	1.95	0.48
1:F:6355:PHE:CD1	1:F:6360:PRO:HG3	2.48	0.48
1:A:1038:VAL:HG21	1:A:1049:ILE:HD12	1.95	0.48
1:C:3290:THR:OG1	1:C:3293:GLU:HB2	2.13	0.48
1:C:3403:TYR:O	1:C:3416:LEU:HD13	2.14	0.48
1:D:4461:PRO:HG2	1:D:4464:VAL:HG23	1.96	0.48
1:D:4040:LEU:HD13	1:D:4155:LEU:HD13	1.95	0.48
1:F:6140:HIS:HD2	1:F:6141:GLY:O	1.96	0.48
1:A:1417:PHE:O	1:A:1420:LEU:HB3	2.13	0.48
1:F:6063:LEU:HD22	1:F:6069:GLN:NE2	2.29	0.48
1:D:4311:ASP:OD1	1:D:4313:ARG:HB2	2.14	0.48
1:A:1381:LEU:HD13	1:A:1417:PHE:CE2	2.49	0.48
1:A:1453:PRO:HA	1:A:1489:GLU:OE1	2.14	0.48
1:D:4359:ILE:HB	1:D:4360:PRO:HD3	1.95	0.48
1:F:6242:ARG:NE	1:F:6504:ALA:O	2.46	0.48
1:A:1237:LYS:HA	1:A:1342:HIS:CE1	2.47	0.47
1:B:2099:GLU:HA	1:B:2107:ASN:HD22	1.79	0.47
1:B:2428:VAL:HG13	1:B:2544:VAL:HG22	1.96	0.47
1:A:1249:VAL:HB	1:A:1433:VAL:HG21	1.96	0.47
1:A:1495:MET:HE3	1:A:1533:THR:HG21	1.95	0.47
7:A:8539:HOH:O	1:C:3292:GLU:HG3	2.14	0.47
1:B:2487:GLU:O	1:B:2491:ARG:HG3	2.13	0.47
1:D:4044:ALA:O	1:D:4046:PRO:HD3	2.14	0.47
1:D:4401:GLU:OE2	1:D:4405:GLY:HA3	2.14	0.47
1:E:5246:GLU:HG2	1:E:5447:TYR:OH	2.14	0.47
1:F:6220:GLU:OE2	1:F:6221:SER:HB2	2.13	0.47
1:F:6242:ARG:HD3	1:F:6503:PHE:O	2.14	0.47
1:C:3317:PRO:O	1:C:3318:LEU:HB3	2.14	0.47
1:C:3343:THR:HB	1:C:3442:ALA:CB	2.17	0.47
1:F:6131:ASN:O	1:F:6132:ARG:HD2	2.13	0.47
1:A:1318:LEU:HD12	1:A:1318:LEU:C	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4478:ALA:N	1:D:4479:PRO:CD	2.77	0.47
1:F:6119:LEU:HD12	1:F:6119:LEU:O	2.14	0.47
1:F:6461:PRO:HG2	1:F:6464:VAL:CG2	2.45	0.47
1:F:6461:PRO:HG2	1:F:6464:VAL:HG23	1.96	0.47
1:B:2348:VAL:O	1:B:2446:MET:HA	2.14	0.47
1:F:6254:VAL:HG21	1:F:6388:LEU:HD23	1.96	0.47
1:A:1242:ARG:HD3	1:A:1503:PHE:O	2.15	0.47
1:A:1383:TRP:CE2	1:A:1393:LYS:HD2	2.50	0.47
1:B:2357:TRP:O	1:B:2360:PRO:HD2	2.13	0.47
1:B:2417:PHE:O	1:B:2420:LEU:HB3	2.15	0.47
1:C:3330:LYS:HG3	1:C:3335:LEU:CD2	2.45	0.47
1:D:4199:ARG:HD3	7:D:8127:HOH:O	2.14	0.47
1:E:5266:GLU:O	1:E:5270:ILE:HG13	2.15	0.47
1:C:3262:LYS:HB3	1:C:3263:PRO:HD3	1.96	0.47
1:D:4140:HIS:HE1	7:D:8029:HOH:O	1.96	0.47
1:D:4338:GLU:C	1:D:4340:ASN:N	2.69	0.47
1:F:6034:LEU:HD13	1:F:6035:GLY:O	2.14	0.47
1:B:2249:VAL:HB	1:B:2433:VAL:HG21	1.96	0.47
1:C:3102:THR:OG1	1:C:3104:ARG:HG2	2.15	0.47
1:C:3330:LYS:HG3	1:C:3335:LEU:HD21	1.97	0.47
1:F:6246:GLU:HG2	1:F:6447:TYR:OH	2.15	0.47
1:C:3126:ASP:H	1:C:3131:ASN:HD21	1.61	0.46
1:A:1105:LYS:HG3	1:A:1481:LEU:O	2.15	0.46
1:B:2136:MET:HB3	1:B:2218:PHE:CE1	2.50	0.46
1:B:2140:HIS:HE1	7:B:8130:HOH:O	1.97	0.46
1:D:4279:SER:N	5:F:682:SIA:H111	2.23	0.46
1:D:4023:PRO:CB	1:D:4034:LEU:HD21	2.40	0.46
1:E:5238:ASN:HB2	7:E:8004:HOH:O	2.15	0.46
1:F:6420:LEU:HD12	1:F:6420:LEU:C	2.35	0.46
1:A:1040:LEU:HD13	1:A:1155:LEU:HD13	1.96	0.46
1:B:2311:ASP:OD1	1:B:2313:ARG:HB2	2.15	0.46
1:D:4352:LYS:HD3	1:D:4450:GLN:NE2	2.18	0.46
1:E:5420:LEU:CD1	1:E:5547:TRP:CZ2	2.98	0.46
1:A:1079:ASN:HB2	5:A:182:SIA:H112	1.96	0.46
1:E:5521:ASN:HB2	7:E:8327:HOH:O	2.16	0.46
1:F:6478:ALA:HB3	1:F:6479:PRO:HD3	1.98	0.46
1:A:1102:THR:OG1	1:A:1104:ARG:HG2	2.16	0.46
1:C:3138:TRP:CZ3	1:C:3219:GLY:HA2	2.51	0.46
1:C:3355:PHE:HD1	1:C:3418:LEU:HD22	1.80	0.46
1:A:1540:LYS:O	1:A:1544:VAL:HG23	2.15	0.46
1:B:2220:GLU:HA	1:B:2246:GLU:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4268:ILE:HG12	1:D:4301:MET:CE	2.46	0.46
1:F:6074:TRP:CD2	1:F:6078:LYS:HE2	2.51	0.46
1:A:1257:LYS:NZ	7:A:8045:HOH:O	2.49	0.46
1:A:1455:PHE:CD2	1:A:1482:LYS:HD3	2.51	0.46
1:C:3339:ARG:HD2	1:C:3440:ALA:HA	1.97	0.46
1:C:3526:TYR:CE2	1:C:3539:LEU:HB2	2.50	0.46
1:D:4357:TRP:CD1	1:D:4461:PRO:HD2	2.51	0.46
4:F:679:NAG:C7	4:F:679:NAG:O3	2.64	0.46
1:B:2048:ALA:HB3	1:B:2123:THR:HG23	1.97	0.46
1:B:2353:GLN:NE2	1:B:2465:ILE:H	2.13	0.46
1:D:4103:ASN:ND2	1:D:4481:LEU:HD12	2.31	0.46
1:D:4257:LYS:NZ	7:D:8035:HOH:O	2.46	0.46
1:A:1336:GLN:NE2	1:A:1433:VAL:HA	2.31	0.45
1:A:1349:GLY:HA3	1:A:1447:TYR:CE1	2.51	0.45
1:C:3120:ASN:HB2	1:C:3167:THR:OG1	2.16	0.45
1:C:3206:ALA:HA	1:C:3210:GLY:O	2.16	0.45
1:D:4386:TYR:N	1:D:4387:PRO:HD2	2.31	0.45
5:E:582:SIA:H6	5:E:582:SIA:C11	2.44	0.45
1:A:1311:ASP:OD1	1:A:1313:ARG:HB2	2.17	0.45
1:B:2359:ILE:HB	1:B:2360:PRO:HD3	1.97	0.45
1:B:2423:ASP:O	1:B:2428:VAL:HG23	2.16	0.45
1:C:3091:PRO:O	1:C:3095:GLN:HG3	2.17	0.45
1:E:5311:ASP:OD1	1:E:5313:ARG:HB2	2.16	0.45
1:E:5447:TYR:HB3	1:E:5517:TRP:CZ2	2.51	0.45
1:F:6547:TRP:CZ3	1:F:6550:LEU:HD23	2.51	0.45
1:A:1357:TRP:CD1	1:A:1461:PRO:HD2	2.51	0.45
1:B:2447:TYR:HB3	1:B:2517:TRP:CZ2	2.51	0.45
1:D:4024:PRO:HD3	1:D:4037:PHE:CE1	2.51	0.45
1:F:6089:GLN:HB2	1:F:6146:VAL:HG12	1.99	0.45
1:F:6467:ASP:N	1:F:6470:ASP:OD2	2.48	0.45
1:A:1428:VAL:HB	1:A:1429:PRO:HD3	1.99	0.45
1:A:1478:ALA:N	1:A:1479:PRO:CD	2.79	0.45
1:D:4104:ARG:NH1	1:D:4153:ASP:HB2	2.32	0.45
1:D:4105:LYS:HE3	1:D:4481:LEU:O	2.17	0.45
1:E:5235:LEU:HD12	1:E:5327:LEU:HA	1.99	0.45
1:A:1234:PRO:O	1:A:1237:LYS:HG2	2.16	0.45
1:B:2102:THR:OG1	1:B:2104:ARG:HG2	2.17	0.45
1:C:3218:PHE:CB	1:C:3244:ILE:HB	2.46	0.45
1:C:3271:THR:HG22	1:C:3297:THR:HG23	1.99	0.45
1:C:3249:VAL:HG23	1:C:3251:LEU:H	1.82	0.45
1:D:4342:HIS:O	1:D:4342:HIS:CD2	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5268:ILE:HG12	1:E:5301:MET:HE2	1.99	0.45
1:F:6316:GLN:HE21	1:F:6316:GLN:HB2	1.61	0.45
1:F:6456:SER:HB3	1:F:6460:LYS:HD3	1.99	0.45
1:C:3130:LYS:HD3	1:C:3132:ARG:CZ	2.47	0.44
1:C:3161:GLU:OE2	1:C:3498:LYS:HG2	2.16	0.44
1:C:3518:PRO:HD3	1:C:3535:ALA:HB2	1.99	0.44
1:D:4074:TRP:CD2	1:D:4078:LYS:HE2	2.52	0.44
1:E:5493:SER:O	1:E:5497:MET:HG3	2.16	0.44
1:A:1450:GLN:CD	7:A:8158:HOH:O	2.56	0.44
1:B:2100:LEU:HD13	1:B:2358:LEU:HD12	1.98	0.44
1:D:4026:VAL:HG13	1:D:4207:SER:HB3	1.99	0.44
1:E:5417:PHE:O	1:E:5420:LEU:HB3	2.17	0.44
1:F:6190:GLY:O	1:F:6194:GLN:HG3	2.17	0.44
1:C:3339:ARG:CD	1:C:3440:ALA:HA	2.48	0.44
1:C:3461:PRO:HG2	1:C:3464:VAL:CG2	2.47	0.44
1:E:5200:TRP:HA	7:E:8785:HOH:O	2.17	0.44
1:A:1461:PRO:HG2	1:A:1464:VAL:HG21	2.00	0.44
1:D:4162:ASN:HD22	1:D:4162:ASN:HA	1.69	0.44
1:F:6132:ARG:O	1:F:6211:ASN:HB2	2.18	0.44
1:F:6258:LYS:HZ3	1:F:6333:GLU:CD	2.20	0.44
1:B:2074:TRP:CD2	1:B:2078:LYS:HE2	2.52	0.44
1:B:2242:ARG:HD3	1:B:2503:PHE:O	2.18	0.44
5:B:282:SIA:C11	1:C:3262:LYS:HZ3	2.30	0.44
1:D:4495:MET:HE3	1:D:4533:THR:HG21	1.99	0.44
1:E:5097:LEU:HD23	1:E:5146:VAL:HG23	1.99	0.44
1:E:5414:LYS:O	1:E:5418:LEU:HG	2.17	0.44
1:B:2143:GLY:O	1:B:2144:LEU:HB2	2.17	0.44
1:C:3218:PHE:HB2	1:C:3244:ILE:HB	2.00	0.44
1:C:3241:HIS:C	1:C:3242:ARG:HG3	2.38	0.44
1:C:3479:PRO:HG2	1:C:3493:SER:HB2	1.99	0.44
1:D:4355:PHE:CD1	1:D:4360:PRO:HG3	2.52	0.44
1:E:5105:LYS:HG3	1:E:5106:GLU:N	2.28	0.44
1:C:3244:ILE:HG12	1:C:3347:MET:HB3	1.98	0.44
1:D:4309:GLN:HE21	1:D:4309:GLN:HB3	1.55	0.44
4:A:179:NAG:C1	7:A:8049:HOH:O	2.66	0.43
5:B:282:SIA:H113	5:B:282:SIA:H4	2.00	0.43
1:D:4052:GLY:O	5:D:482:SIA:H92	2.18	0.43
1:D:4252:THR:HG22	1:D:4254:VAL:HG12	2.00	0.43
1:D:4318:LEU:HD12	1:D:4318:LEU:C	2.38	0.43
1:E:5100:LEU:HD13	1:E:5358:LEU:HD11	1.99	0.43
1:E:5357:TRP:O	1:E:5360:PRO:HD2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1351:ASN:HB3	1:A:1466:GLY:O	2.19	0.43
1:F:6258:LYS:HE2	1:F:6331:THR:HB	1.99	0.43
1:F:6495:MET:HG3	1:F:6514:LEU:HD22	1.99	0.43
1:A:1394:GLU:O	1:A:1397:PRO:HD2	2.18	0.43
1:D:4242:ARG:HD3	1:D:4503:PHE:O	2.19	0.43
1:E:5258:LYS:HD2	1:E:5258:LYS:O	2.18	0.43
1:E:5447:TYR:CD2	1:E:5447:TYR:C	2.91	0.43
4:E:579:NAG:H83	5:E:582:SIA:H31	2.00	0.43
1:B:2029:VAL:HG23	1:B:2204:ASN:OD1	2.17	0.43
1:C:3023:PRO:HB3	1:C:3034:LEU:HD21	2.00	0.43
1:E:5126:ASP:OD2	1:E:5128:THR:OG1	2.36	0.43
1:F:6145:MET:SD	1:F:6173:GLY:HA2	2.58	0.43
1:C:3246:GLU:HG2	1:C:3447:TYR:OH	2.19	0.43
1:B:2437:HIS:HE1	7:B:8097:HOH:O	2.00	0.43
1:C:3480:PHE:CZ	1:C:3490:ILE:HG23	2.53	0.43
1:D:4527:LEU:HD11	1:D:4533:THR:HG22	2.00	0.43
1:F:6338:GLU:C	1:F:6340:ASN:N	2.72	0.43
1:E:5038:VAL:HG21	1:E:5049:ILE:HD12	2.00	0.43
1:E:5161:GLU:OE2	1:E:5498:LYS:HG2	2.18	0.43
1:F:6048:ALA:HB3	1:F:6123:THR:HG23	2.01	0.43
1:F:6338:GLU:HG2	1:F:6340:ASN:ND2	2.30	0.43
1:F:6414:LYS:HE3	1:F:6414:LYS:HB3	1.93	0.43
5:A:182:SIA:H113	5:A:182:SIA:O4	2.19	0.43
1:B:2161:GLU:OE2	1:B:2498:LYS:HG2	2.19	0.43
1:C:3403:TYR:CD1	1:C:3420:LEU:HD22	2.53	0.43
1:D:4275:LYS:HG3	7:D:8565:HOH:O	2.17	0.43
1:E:5330:LYS:HG3	1:E:5335:LEU:HG	2.00	0.43
1:B:2197:ALA:O	1:B:2201:VAL:HG23	2.19	0.43
1:B:2366:TYR:HA	1:B:2367:PRO:HD3	1.80	0.43
1:B:2447:TYR:CD2	1:B:2447:TYR:C	2.92	0.43
1:B:2501:ALA:O	1:B:2505:ARG:HG2	2.18	0.43
1:D:4404:LEU:C	1:D:4406:GLY:H	2.23	0.43
1:E:5242:ARG:HG2	1:E:5242:ARG:NH1	2.28	0.43
1:A:1312:PRO:HG3	1:A:1384:LYS:HD3	2.01	0.43
1:B:2153:ASP:OD2	1:B:2155:LEU:HB2	2.19	0.43
1:B:2268:ILE:HG12	1:B:2301:MET:CE	2.49	0.43
1:D:4283:VAL:O	1:D:4287:ARG:HG3	2.19	0.43
1:A:1252:THR:HG22	1:A:1254:VAL:HG12	2.00	0.42
1:B:2246:GLU:HG2	1:B:2447:TYR:OH	2.18	0.42
1:A:1528:GLN:O	1:A:1533:THR:HA	2.19	0.42
1:C:3036:LYS:HD3	7:C:8059:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3114:GLU:CG	1:C:3291:GLU:HG3	2.48	0.42
1:E:5044:ALA:O	1:E:5046:PRO:HD3	2.19	0.42
1:E:5264:LEU:O	1:E:5268:ILE:HG13	2.18	0.42
1:F:6205:ILE:HD12	1:F:6205:ILE:HA	1.84	0.42
1:F:6313:ARG:HG2	1:F:6386:TYR:CE2	2.55	0.42
1:A:1526:TYR:CD2	1:A:1539:LEU:HB2	2.54	0.42
1:B:2242:ARG:HG2	1:B:2242:ARG:NH1	2.33	0.42
1:C:3301:MET:HB2	1:C:3303:PHE:CE1	2.55	0.42
1:A:1205:ILE:HA	1:A:1205:ILE:HD12	1.86	0.42
1:A:1218:PHE:CB	1:A:1244:ILE:HB	2.50	0.42
1:A:1355:PHE:CE1	1:A:1360:PRO:HG3	2.54	0.42
1:B:2343:THR:HB	1:B:2442:ALA:HB2	2.01	0.42
1:B:2420:LEU:CD1	1:B:2547:TRP:HZ2	2.32	0.42
1:B:2384:LYS:NZ	7:B:8272:HOH:O	2.53	0.42
1:D:4220:GLU:OE2	1:D:4221:SER:HB2	2.20	0.42
1:E:5142:GLY:N	3:E:1:GD7:O11	2.44	0.42
1:F:6238:ASN:N	7:F:8536:HOH:O	2.51	0.42
1:F:6338:GLU:C	1:F:6340:ASN:H	2.22	0.42
1:A:1349:GLY:HA3	1:A:1447:TYR:CZ	2.54	0.42
1:A:1461:PRO:HG2	1:A:1464:VAL:CG2	2.49	0.42
1:A:1553:LYS:HB2	1:A:1553:LYS:HZ2	1.84	0.42
1:A:1047:VAL:HG21	1:A:1155:LEU:HD23	2.01	0.42
1:A:1263:PRO:O	1:A:1267:GLN:HG3	2.20	0.42
1:C:3139:ILE:O	1:C:3223:GLY:HA3	2.20	0.42
1:D:4041:GLU:HG3	7:D:8132:HOH:O	2.19	0.42
1:D:4310:GLY:O	1:D:4312:PRO:HD3	2.20	0.42
1:D:4268:ILE:HG12	1:D:4301:MET:HE2	2.01	0.42
1:F:6315:SER:HB2	7:F:8811:HOH:O	2.18	0.42
1:F:6518:PRO:HD3	1:F:6535:ALA:HB2	2.01	0.42
1:B:2264:LEU:O	1:B:2268:ILE:HG13	2.19	0.42
1:B:2382:LEU:HD12	1:B:2382:LEU:HA	1.88	0.42
1:C:3143:GLY:O	1:C:3144:LEU:HB2	2.19	0.42
1:D:4393:LYS:HA	1:D:4396:ILE:HG12	2.02	0.42
1:E:5250:ALA:HB1	1:E:5332:PRO:HB3	2.02	0.42
1:E:5427:GLY:O	1:E:5431:VAL:HG23	2.19	0.42
1:F:6292:GLU:CD	1:F:6292:GLU:H	2.23	0.42
1:A:1257:LYS:NZ	1:A:1318:LEU:O	2.42	0.42
5:A:182:SIA:H92	7:A:8253:HOH:O	2.19	0.42
1:B:2132:ARG:HG3	1:B:2211:ASN:HB2	2.01	0.42
1:B:2268:ILE:HG12	1:B:2301:MET:HE2	2.02	0.42
1:B:2336:GLN:O	1:B:2339:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3025:VAL:HG22	1:C:3034:LEU:HD23	2.01	0.42
1:E:5221:SER:HA	1:E:5247:SER:O	2.20	0.42
1:C:3074:TRP:CD2	1:C:3078:LYS:HE2	2.54	0.41
1:C:3528:GLN:O	1:C:3533:THR:HA	2.19	0.41
1:D:4450:GLN:CD	7:D:8108:HOH:O	2.58	0.41
1:F:6066:THR:HG23	1:F:6287:ARG:HH21	1.84	0.41
1:F:6114:GLU:HG3	1:F:6291:GLU:OE2	2.20	0.41
1:F:6206:ALA:HA	1:F:6210:GLY:O	2.19	0.41
1:C:3103:ASN:ND2	1:C:3476:PHE:HB3	2.35	0.41
1:A:1038:VAL:CG2	1:A:1049:ILE:HD12	2.49	0.41
1:B:2023:PRO:HB2	1:B:2034:LEU:CD2	2.47	0.41
1:B:2278:THR:OG1	1:B:2281:VAL:HG23	2.20	0.41
5:B:282:SIA:C11	1:C:3262:LYS:HZ1	2.32	0.41
1:D:4478:ALA:HB3	1:D:4479:PRO:HD3	2.02	0.41
1:E:5461:PRO:HG2	1:E:5464:VAL:HG23	2.01	0.41
1:A:1283:VAL:O	1:A:1287:ARG:HG3	2.21	0.41
1:C:3381:LEU:HD13	1:C:3417:PHE:CE2	2.55	0.41
1:D:4220:GLU:HA	1:D:4246:GLU:O	2.20	0.41
1:D:4364:MET:SD	1:D:4388:LEU:HD11	2.60	0.41
1:D:4498:LYS:HB3	1:D:4514:LEU:HD11	2.01	0.41
1:E:5205:ILE:HA	1:E:5205:ILE:HD12	1.84	0.41
1:C:3461:PRO:HG2	1:C:3464:VAL:HG23	2.01	0.41
1:D:4396:ILE:HB	1:D:4397:PRO:CD	2.44	0.41
1:E:5461:PRO:HG2	1:E:5464:VAL:CG2	2.50	0.41
1:F:6079:ASN:HB2	5:F:682:SIA:C1	2.51	0.41
1:A:1105:LYS:HE3	1:A:1481:LEU:O	2.20	0.41
1:A:1526:TYR:CE2	1:A:1539:LEU:HB2	2.55	0.41
1:C:3296:GLU:O	1:C:3300:LYS:HG3	2.20	0.41
1:C:3540:LYS:O	1:C:3544:VAL:HG23	2.20	0.41
1:E:5119:LEU:HD12	1:E:5119:LEU:O	2.19	0.41
1:F:6241:HIS:C	1:F:6242:ARG:CG	2.89	0.41
1:A:1252:THR:HG22	1:A:1252:THR:O	2.20	0.41
1:A:1331:THR:OG1	1:A:1334:GLU:HG3	2.20	0.41
1:A:1366:TYR:HA	1:A:1367:PRO:HD3	1.82	0.41
1:C:3456:SER:HB3	1:C:3460:LYS:HD3	2.03	0.41
1:D:4152:TYR:CD1	1:D:4152:TYR:N	2.88	0.41
1:F:6063:LEU:HD22	1:F:6069:GLN:HE22	1.86	0.41
1:F:6309:GLN:HE21	1:F:6309:GLN:HB3	1.47	0.41
1:B:2038:VAL:HG21	1:B:2049:ILE:HD12	2.03	0.41
1:C:3338:GLU:O	1:C:3339:ARG:C	2.59	0.41
1:D:4366:TYR:HA	1:D:4367:PRO:HD3	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5242:ARG:HH11	1:E:5242:ARG:CG	2.29	0.41
1:F:6038:VAL:HG13	7:F:8677:HOH:O	2.19	0.41
1:A:1187:GLY:O	1:A:1188:ASN:HB2	2.21	0.41
1:A:1309:GLN:HE21	1:A:1309:GLN:HB3	1.51	0.41
1:A:1414:LYS:O	1:A:1418:LEU:HG	2.20	0.41
1:B:2022:SER:HA	1:B:2023:PRO:HD3	1.88	0.41
1:B:2316:GLN:HE21	1:B:2316:GLN:HB2	1.64	0.41
1:D:4374:ASP:O	1:D:4375:GLN:C	2.60	0.41
1:D:4526:TYR:CE2	1:D:4539:LEU:HB2	2.56	0.41
1:E:5221:SER:OG	3:E:1:GD7:H41	2.21	0.41
1:E:5237:LYS:O	1:E:5238:ASN:CG	2.59	0.41
1:E:5262:LYS:HB3	1:E:5263:PRO:HD3	2.02	0.41
1:F:6262:LYS:N	1:F:6263:PRO:CD	2.84	0.41
1:F:6294:LEU:HD23	1:F:6294:LEU:HA	1.91	0.41
1:F:6333:GLU:OE1	1:F:6333:GLU:N	2.53	0.41
1:F:6349:GLY:HA3	1:F:6447:TYR:CZ	2.56	0.41
1:A:1283:VAL:HG12	1:A:1287:ARG:NH1	2.36	0.41
1:B:2048:ALA:HB3	1:B:2123:THR:CG2	2.50	0.41
1:B:2130:LYS:NZ	1:B:2130:LYS:HB3	2.36	0.41
1:B:2351:ASN:ND2	1:B:2449:PHE:HB3	2.36	0.41
1:C:3505:ARG:H	1:C:3505:ARG:HG2	1.66	0.41
1:E:5538:LYS:HD2	1:E:5541:ASP:OD2	2.20	0.41
1:F:6237:LYS:O	1:F:6238:ASN:CG	2.59	0.41
1:A:1104:ARG:HD3	7:A:8963:HOH:O	2.19	0.40
1:A:1316:GLN:HA	1:A:1317:PRO:HD2	1.98	0.40
1:C:3332:PRO:O	1:C:3336:GLN:HG3	2.21	0.40
1:D:4431:VAL:HG21	1:D:4540:LYS:HB2	2.04	0.40
1:E:5119:LEU:HD12	1:E:5119:LEU:C	2.41	0.40
1:A:1336:GLN:HE22	1:A:1433:VAL:HA	1.85	0.40
1:B:2268:ILE:HD11	1:B:2319:LEU:HD21	2.04	0.40
1:C:3349:GLY:HA3	1:C:3447:TYR:CE1	2.56	0.40
1:D:4349:GLY:HA3	1:D:4447:TYR:CZ	2.56	0.40
1:D:4420:LEU:CD1	1:D:4547:TRP:HZ2	2.35	0.40
1:D:4420:LEU:CD1	1:D:4547:TRP:CZ2	3.04	0.40
1:E:5268:ILE:HG12	1:E:5301:MET:CE	2.50	0.40
1:E:5366:TYR:HA	1:E:5367:PRO:HD3	1.83	0.40
1:F:6442:ALA:HA	1:F:6443:PRO:HD3	1.96	0.40
1:C:3271:THR:CG2	1:C:3297:THR:HG23	2.52	0.40
1:D:4357:TRP:O	1:D:4360:PRO:HD2	2.22	0.40
1:E:5198:LEU:HB3	1:E:5239:LEU:HB3	2.03	0.40
1:F:6130:LYS:O	1:F:6130:LYS:CD	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5471:GLU:OE2	1:E:5471:GLU:N	2.53	0.40
1:F:6349:GLY:HA3	1:F:6447:TYR:CE1	2.57	0.40
1:B:2467:ASP:N	1:B:2470:ASP:OD2	2.49	0.40
1:E:5215:VAL:H	1:E:5241:HIS:CD2	2.16	0.40
1:F:6138:TRP:CZ3	1:F:6219:GLY:HA2	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	530/532 (100%)	497 (94%)	29 (6%)	4 (1%)	19	43
1	B	529/532 (99%)	495 (94%)	34 (6%)	0	100	100
1	C	529/532 (99%)	502 (95%)	25 (5%)	2 (0%)	34	60
1	D	530/532 (100%)	496 (94%)	32 (6%)	2 (0%)	34	60
1	E	529/532 (99%)	498 (94%)	27 (5%)	4 (1%)	19	43
1	F	529/532 (99%)	500 (94%)	28 (5%)	1 (0%)	47	73
All	All	3176/3192 (100%)	2988 (94%)	175 (6%)	13 (0%)	34	60

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	5238	ASN
1	F	6238	ASN
1	C	3076	PHE
1	C	3238	ASN
1	D	4253	SER
1	D	4375	GLN
1	E	5253	SER

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Mol	Chain	Res	Type
1	E	5341	PHE
1	A	1253	SER
1	A	1341	PHE
1	A	1375	GLN
1	A	1238	ASN
1	E	5367	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	448/448 (100%)	430 (96%)	18 (4%)	31	60
1	B	447/448 (100%)	432 (97%)	15 (3%)	37	66
1	C	447/448 (100%)	432 (97%)	15 (3%)	37	66
1	D	448/448 (100%)	426 (95%)	22 (5%)	25	52
1	E	447/448 (100%)	433 (97%)	14 (3%)	40	69
1	F	447/448 (100%)	435 (97%)	12 (3%)	44	74
All	All	2684/2688 (100%)	2588 (96%)	96 (4%)	35	64

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1079	ASN
1	A	1104	ARG
1	A	1130	LYS
1	A	1132	ARG
1	A	1155	LEU
1	A	1162	ASN
1	A	1218	PHE
1	A	1220	GLU
1	A	1258	LYS
1	A	1264	LEU
1	A	1309	GLN
1	A	1316	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1342	HIS
1	A	1366	TYR
1	A	1381	LEU
1	A	1414	LYS
1	A	1420	LEU
1	A	1483	GLU
1	B	2104	ARG
1	B	2130	LYS
1	B	2132	ARG
1	B	2155	LEU
1	B	2218	PHE
1	B	2220	GLU
1	B	2258	LYS
1	B	2264	LEU
1	B	2292	GLU
1	B	2299	LEU
1	B	2309	GLN
1	B	2316	GLN
1	B	2330	LYS
1	B	2499	PHE
1	B	2500	TRP
1	C	3092	LYS
1	C	3130	LYS
1	C	3155	LEU
1	C	3218	PHE
1	C	3220	GLU
1	C	3258	LYS
1	C	3264	LEU
1	C	3309	GLN
1	C	3316	GLN
1	C	3330	LYS
1	C	3358	LEU
1	C	3381	LEU
1	C	3414	LYS
1	C	3420	LEU
1	C	3500	TRP
1	D	4021	SER
1	D	4079	ASN
1	D	4130	LYS
1	D	4132	ARG
1	D	4155	LEU
1	D	4162	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	4218	PHE
1	D	4220	GLU
1	D	4242	ARG
1	D	4258	LYS
1	D	4264	LEU
1	D	4299	LEU
1	D	4309	GLN
1	D	4316	GLN
1	D	4342	HIS
1	D	4366	TYR
1	D	4372	GLN
1	D	4414	LYS
1	D	4491	ARG
1	D	4498	LYS
1	D	4512	GLU
1	D	4553	LYS
1	E	5130	LYS
1	E	5132	ARG
1	E	5155	LEU
1	E	5218	PHE
1	E	5220	GLU
1	E	5258	LYS
1	E	5264	LEU
1	E	5309	GLN
1	E	5316	GLN
1	E	5366	TYR
1	E	5410	THR
1	E	5414	LYS
1	E	5499	PHE
1	E	5500	TRP
1	F	6130	LYS
1	F	6155	LEU
1	F	6218	PHE
1	F	6220	GLU
1	F	6264	LEU
1	F	6299	LEU
1	F	6309	GLN
1	F	6316	GLN
1	F	6381	LEU
1	F	6420	LEU
1	F	6499	PHE
1	F	6500	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1030	HIS
1	A	1131	ASN
1	A	1140	HIS
1	A	1162	ASN
1	A	1238	ASN
1	A	1241	HIS
1	A	1309	GLN
1	A	1316	GLN
1	A	1336	GLN
1	A	1351	ASN
1	A	1375	GLN
1	A	1436	ASN
1	A	1450	GLN
1	A	1537	GLN
1	B	2045	GLN
1	B	2107	ASN
1	B	2131	ASN
1	B	2140	HIS
1	B	2241	HIS
1	B	2309	GLN
1	B	2316	GLN
1	B	2351	ASN
1	B	2353	GLN
1	B	2375	GLN
1	B	2436	ASN
1	B	2532	ASN
1	B	2537	GLN
1	C	3030	HIS
1	C	3045	GLN
1	C	3069	GLN
1	C	3107	ASN
1	C	3131	ASN
1	C	3140	HIS
1	C	3241	HIS
1	C	3309	GLN
1	C	3351	ASN
1	C	3436	ASN
1	C	3450	GLN
1	C	3537	GLN
1	D	4069	GLN
1	D	4140	HIS

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Mol	Chain	Res	Type
1	D	4162	ASN
1	D	4241	HIS
1	D	4309	GLN
1	D	4316	GLN
1	D	4351	ASN
1	D	4375	GLN
1	D	4450	GLN
1	D	4537	GLN
1	E	5107	ASN
1	E	5131	ASN
1	E	5140	HIS
1	E	5162	ASN
1	E	5241	HIS
1	E	5309	GLN
1	E	5351	ASN
1	E	5436	ASN
1	E	5534	GLN
1	E	5537	GLN
1	F	6045	GLN
1	F	6069	GLN
1	F	6107	ASN
1	F	6131	ASN
1	F	6140	HIS
1	F	6241	HIS
1	F	6288	GLN
1	F	6309	GLN
1	F	6340	ASN
1	F	6342	HIS
1	F	6351	ASN
1	F	6372	GLN
1	F	6436	ASN
1	F	6537	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates i

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GLC	G	1	2	11,11,12	1.65	2 (18%)	15,15,17	0.95	0
2	FRU	G	2	2	11,12,12	1.60	1 (9%)	10,18,18	1.07	1 (10%)
2	GLC	H	1	2	11,11,12	1.67	3 (27%)	15,15,17	1.02	1 (6%)
2	FRU	H	2	2	11,12,12	1.51	1 (9%)	10,18,18	0.89	0
2	GLC	I	1	2	11,11,12	1.53	2 (18%)	15,15,17	1.01	1 (6%)
2	FRU	I	2	2	11,12,12	1.49	1 (9%)	10,18,18	0.94	0
2	GLC	J	1	2	11,11,12	1.59	2 (18%)	15,15,17	0.99	1 (6%)
2	FRU	J	2	2	11,12,12	1.70	1 (9%)	10,18,18	0.75	0
2	GLC	K	1	2	11,11,12	1.65	2 (18%)	15,15,17	1.01	1 (6%)
2	FRU	K	2	2	11,12,12	1.52	1 (9%)	10,18,18	0.79	0
2	GLC	L	1	2	11,11,12	1.54	1 (9%)	15,15,17	1.07	1 (6%)
2	FRU	L	2	2	11,12,12	1.39	1 (9%)	10,18,18	1.05	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	G	1	2	-	2/2/19/22	0/1/1/1
2	FRU	G	2	2	-	5/5/24/24	0/1/1/1
2	GLC	H	1	2	-	2/2/19/22	0/1/1/1
2	FRU	H	2	2	-	1/5/24/24	0/1/1/1
2	GLC	I	1	2	-	0/2/19/22	0/1/1/1
2	FRU	I	2	2	-	0/5/24/24	0/1/1/1
2	GLC	J	1	2	-	0/2/19/22	0/1/1/1
2	FRU	J	2	2	-	2/5/24/24	0/1/1/1
2	GLC	K	1	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FRU	K	2	2	-	2/5/24/24	0/1/1/1
2	GLC	L	1	2	-	0/2/19/22	0/1/1/1
2	FRU	L	2	2	-	0/5/24/24	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	2	FRU	O2-C2	5.37	1.49	1.40
2	G	2	FRU	O2-C2	5.11	1.49	1.40
2	K	2	FRU	O2-C2	4.74	1.48	1.40
2	H	2	FRU	O2-C2	4.67	1.48	1.40
2	I	2	FRU	O2-C2	4.58	1.48	1.40
2	L	2	FRU	O2-C2	4.37	1.48	1.40
2	H	1	GLC	O5-C1	3.84	1.49	1.43
2	L	1	GLC	O5-C1	3.72	1.49	1.43
2	K	1	GLC	O5-C1	3.68	1.49	1.43
2	J	1	GLC	O5-C1	3.58	1.49	1.43
2	I	1	GLC	O5-C1	3.48	1.49	1.43
2	G	1	GLC	O5-C1	3.46	1.49	1.43
2	G	1	GLC	C2-C3	2.65	1.56	1.52
2	K	1	GLC	C2-C3	2.20	1.55	1.52
2	I	1	GLC	C2-C3	2.20	1.55	1.52
2	J	1	GLC	C2-C3	2.12	1.55	1.52
2	H	1	GLC	C2-C3	2.05	1.55	1.52
2	H	1	GLC	O5-C5	2.03	1.47	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1	GLC	C1-O5-C5	2.32	115.33	112.19
2	K	1	GLC	C1-O5-C5	2.20	115.18	112.19
2	G	2	FRU	O1-C1-C2	-2.18	107.24	111.86
2	H	1	GLC	C1-O5-C5	2.13	115.08	112.19
2	J	1	GLC	C1-O5-C5	2.10	115.04	112.19
2	I	1	GLC	C1-O5-C5	2.06	114.99	112.19

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	2	FRU	O1-C1-C2-O2

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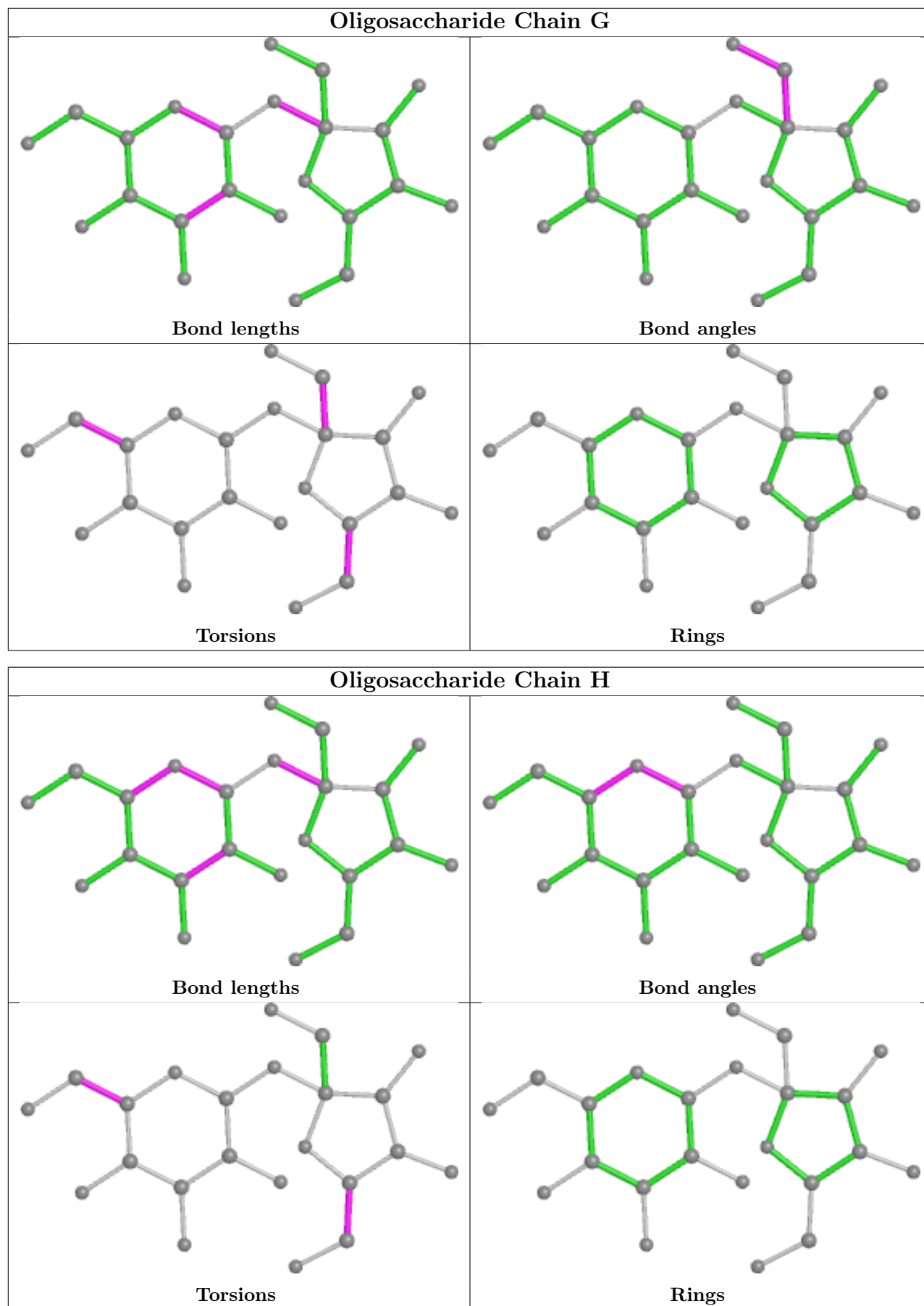
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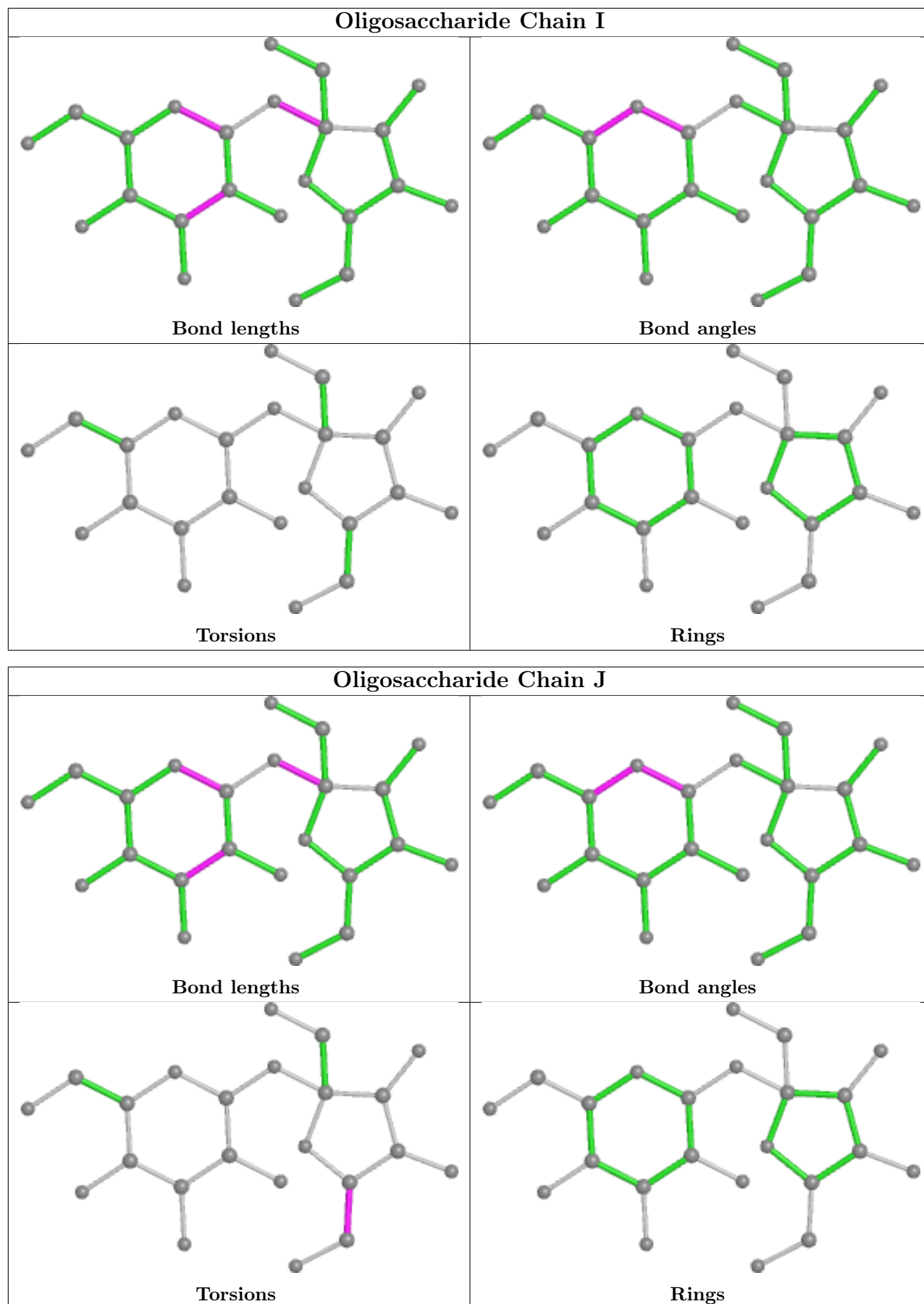
Mol	Chain	Res	Type	Atoms
2	G	2	FRU	O5-C5-C6-O6
2	J	2	FRU	O5-C5-C6-O6
2	J	2	FRU	C4-C5-C6-O6
2	G	2	FRU	C4-C5-C6-O6
2	K	1	GLC	O5-C5-C6-O6
2	K	1	GLC	C4-C5-C6-O6
2	H	1	GLC	C4-C5-C6-O6
2	H	1	GLC	O5-C5-C6-O6
2	G	1	GLC	O5-C5-C6-O6
2	G	2	FRU	O1-C1-C2-C3
2	K	2	FRU	O5-C5-C6-O6
2	K	2	FRU	C4-C5-C6-O6
2	G	2	FRU	O1-C1-C2-O5
2	G	1	GLC	C4-C5-C6-O6
2	H	2	FRU	O5-C5-C6-O6

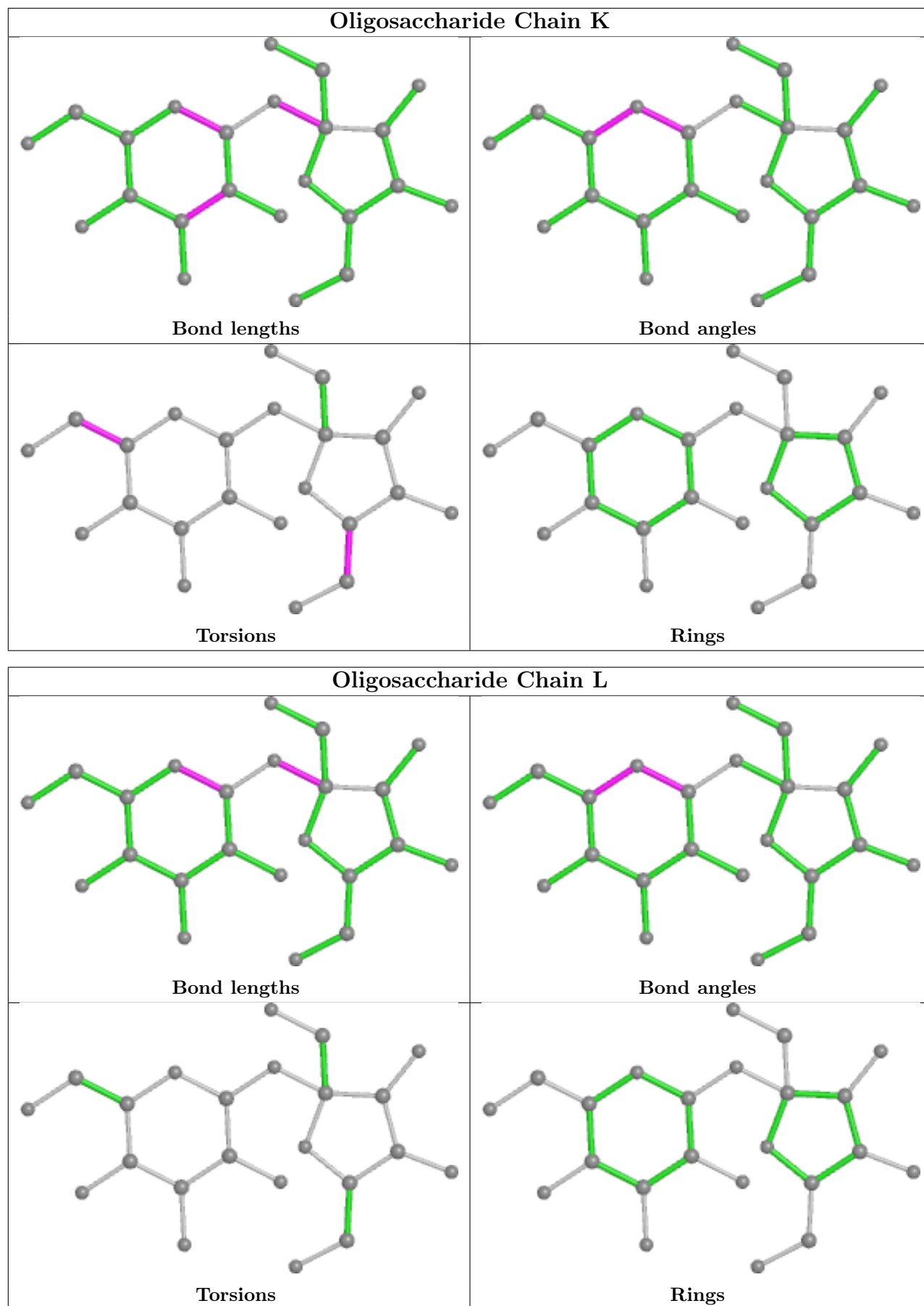
There are no ring outliers.

No monomer is involved in short contacts.

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







## 5.6 Ligand geometry

30 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	F	679	1	14,14,15	0.64	0	17,19,21	0.76	0
4	NAG	C	379	1	14,14,15	0.66	0	17,19,21	0.77	0
3	GD7	A	1	1	6,9,9	0.83	0	7,13,13	0.14	0
6	SO4	A	185	-	4,4,4	0.27	0	6,6,6	0.06	0
6	SO4	A	284	-	4,4,4	0.26	0	6,6,6	0.05	0
3	GD7	D	1	1	6,9,9	0.86	0	7,13,13	0.13	0
6	SO4	C	184	-	4,4,4	0.26	0	6,6,6	0.08	0
6	SO4	F	685	-	4,4,4	0.28	0	6,6,6	0.06	0
5	SIA	D	482	-	21,21,21	0.87	1 (4%)	25,31,31	1.04	2 (8%)
3	GD7	C	1	1	6,9,9	0.83	0	7,13,13	0.24	0
4	NAG	B	279	1	14,14,15	0.74	0	17,19,21	0.73	0
4	NAG	D	479	1	14,14,15	0.80	1 (7%)	17,19,21	0.65	0
6	SO4	F	684	-	4,4,4	0.25	0	6,6,6	0.05	0
3	GD7	E	1	1	6,9,9	0.81	0	7,13,13	0.20	0
6	SO4	F	485	-	4,4,4	0.27	0	6,6,6	0.06	0
6	SO4	D	484	-	4,4,4	0.27	0	6,6,6	0.05	0
5	SIA	F	682	-	21,21,21	0.98	0	25,31,31	0.97	1 (4%)
4	NAG	A	179	1	14,14,15	0.78	1 (7%)	17,19,21	0.59	0
6	SO4	C	384	-	4,4,4	0.26	0	6,6,6	0.05	0
3	GD7	B	1	1	6,9,9	0.86	0	7,13,13	0.29	0
6	SO4	E	584	-	4,4,4	0.27	0	6,6,6	0.06	0
5	SIA	E	582	-	21,21,21	0.99	0	25,31,31	1.20	3 (12%)
5	SIA	A	182	-	21,21,21	0.94	1 (4%)	25,31,31	0.99	2 (8%)
5	SIA	C	382	-	21,21,21	0.84	0	25,31,31	0.99	2 (8%)
3	GD7	F	1	1	6,9,9	0.83	0	7,13,13	0.26	0
6	SO4	B	285	-	4,4,4	0.25	0	6,6,6	0.12	0
6	SO4	B	385	-	4,4,4	0.26	0	6,6,6	0.07	0
4	NAG	E	579	1	14,14,15	0.57	0	17,19,21	0.67	0
6	SO4	D	585	-	4,4,4	0.27	0	6,6,6	0.05	0
5	SIA	B	282	-	21,21,21	0.98	1 (4%)	25,31,31	1.18	3 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	279	1	-	6/6/23/26	0/1/1/1
4	NAG	F	679	1	-	6/6/23/26	0/1/1/1
5	SIA	D	482	-	-	7/20/38/38	0/1/1/1
3	GD7	B	1	1	-	0/6/10/10	-
4	NAG	D	479	1	-	6/6/23/26	0/1/1/1
4	NAG	C	379	1	-	6/6/23/26	0/1/1/1
3	GD7	A	1	1	-	0/6/10/10	-
3	GD7	E	1	1	-	0/6/10/10	-
5	SIA	E	582	-	-	9/20/38/38	0/1/1/1
4	NAG	E	579	1	-	6/6/23/26	0/1/1/1
5	SIA	B	282	-	-	11/20/38/38	0/1/1/1
5	SIA	A	182	-	-	9/20/38/38	0/1/1/1
3	GD7	D	1	1	-	0/6/10/10	-
5	SIA	F	682	-	-	9/20/38/38	0/1/1/1
4	NAG	A	179	1	-	6/6/23/26	0/1/1/1
5	SIA	C	382	-	-	8/20/38/38	0/1/1/1
3	GD7	F	1	1	-	0/6/10/10	-
3	GD7	C	1	1	-	0/6/10/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	479	NAG	C1-C2	2.44	1.56	1.52
4	A	179	NAG	C1-C2	2.24	1.55	1.52
5	D	482	SIA	O6-C2	2.18	1.45	1.43
5	B	282	SIA	C7-C6	2.09	1.55	1.53
5	A	182	SIA	C3-C2	2.05	1.54	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	682	SIA	O1A-C1-C2	-3.42	118.42	123.59
5	C	382	SIA	O1A-C1-C2	-3.32	118.56	123.59
5	A	182	SIA	O1A-C1-C2	-3.28	118.62	123.59
5	D	482	SIA	O1A-C1-C2	-3.23	118.70	123.59
5	B	282	SIA	O1A-C1-C2	-3.19	118.76	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	582	SIA	O1A-C1-C2	-3.16	118.81	123.59
5	B	282	SIA	O6-C6-C7	2.78	111.58	107.29
5	E	582	SIA	O6-C6-C7	2.77	111.56	107.29
5	B	282	SIA	C3-C2-C1	-2.57	108.22	113.00
5	E	582	SIA	C3-C2-C1	-2.31	108.70	113.00
5	D	482	SIA	C3-C2-C1	-2.18	108.94	113.00
5	A	182	SIA	C3-C2-C1	-2.04	109.20	113.00
5	C	382	SIA	O6-C6-C7	2.00	110.38	107.29

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	179	NAG	C8-C7-N2-C2
4	A	179	NAG	O7-C7-N2-C2
4	B	279	NAG	C8-C7-N2-C2
4	B	279	NAG	O7-C7-N2-C2
4	C	379	NAG	C8-C7-N2-C2
4	C	379	NAG	O7-C7-N2-C2
4	D	479	NAG	C8-C7-N2-C2
4	D	479	NAG	O7-C7-N2-C2
4	E	579	NAG	C8-C7-N2-C2
4	E	579	NAG	O7-C7-N2-C2
4	F	679	NAG	C8-C7-N2-C2
4	F	679	NAG	O7-C7-N2-C2
5	A	182	SIA	O1B-C1-C2-O6
5	A	182	SIA	C5-C6-C7-C8
5	A	182	SIA	C5-C6-C7-O7
5	A	182	SIA	O6-C6-C7-C8
5	A	182	SIA	O6-C6-C7-O7
5	A	182	SIA	C7-C8-C9-O9
5	A	182	SIA	C11-C10-N5-C5
5	A	182	SIA	O10-C10-N5-C5
5	B	282	SIA	C4-C5-N5-C10
5	B	282	SIA	C5-C6-C7-C8
5	B	282	SIA	C5-C6-C7-O7
5	B	282	SIA	O6-C6-C7-C8
5	B	282	SIA	O6-C6-C7-O7
5	B	282	SIA	C6-C7-C8-O8
5	B	282	SIA	O7-C7-C8-O8
5	B	282	SIA	C11-C10-N5-C5
5	B	282	SIA	O10-C10-N5-C5

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Mol	Chain	Res	Type	Atoms
5	C	382	SIA	O1A-C1-C2-O2
5	C	382	SIA	O1A-C1-C2-O6
5	C	382	SIA	O1B-C1-C2-O2
5	C	382	SIA	O1B-C1-C2-O6
5	C	382	SIA	C4-C5-N5-C10
5	C	382	SIA	C5-C6-C7-C8
5	C	382	SIA	C11-C10-N5-C5
5	C	382	SIA	O10-C10-N5-C5
5	D	482	SIA	C11-C10-N5-C5
5	D	482	SIA	O10-C10-N5-C5
5	E	582	SIA	C4-C5-N5-C10
5	E	582	SIA	C5-C6-C7-C8
5	E	582	SIA	C5-C6-C7-O7
5	E	582	SIA	O6-C6-C7-C8
5	E	582	SIA	O6-C6-C7-O7
5	E	582	SIA	C11-C10-N5-C5
5	E	582	SIA	O10-C10-N5-C5
5	F	682	SIA	O1B-C1-C2-C3
5	F	682	SIA	C4-C5-N5-C10
5	F	682	SIA	C11-C10-N5-C5
5	F	682	SIA	O10-C10-N5-C5
4	B	279	NAG	C4-C5-C6-O6
4	B	279	NAG	O5-C5-C6-O6
4	E	579	NAG	C1-C2-N2-C7
5	A	182	SIA	O8-C8-C9-O9
4	E	579	NAG	O5-C5-C6-O6
4	C	379	NAG	O5-C5-C6-O6
4	A	179	NAG	O5-C5-C6-O6
4	D	479	NAG	O5-C5-C6-O6
4	F	679	NAG	O5-C5-C6-O6
4	A	179	NAG	C4-C5-C6-O6
4	A	179	NAG	C1-C2-N2-C7
4	C	379	NAG	C1-C2-N2-C7
4	F	679	NAG	C1-C2-N2-C7
5	B	282	SIA	O7-C7-C8-C9
5	B	282	SIA	C6-C7-C8-C9
5	F	682	SIA	O8-C8-C9-O9
4	C	379	NAG	C4-C5-C6-O6
4	E	579	NAG	C4-C5-C6-O6
4	D	479	NAG	C4-C5-C6-O6
4	F	679	NAG	C4-C5-C6-O6
4	B	279	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
5	F	682	SIA	C7-C8-C9-O9
4	D	479	NAG	C1-C2-N2-C7
5	D	482	SIA	C6-C5-N5-C10
4	F	679	NAG	C3-C2-N2-C7
5	D	482	SIA	O1A-C1-C2-C3
5	D	482	SIA	O1A-C1-C2-O6
5	E	582	SIA	O1A-C1-C2-O6
5	D	482	SIA	O1A-C1-C2-O2
5	F	682	SIA	C5-C6-C7-C8
4	A	179	NAG	C3-C2-N2-C7
4	C	379	NAG	C3-C2-N2-C7
4	E	579	NAG	C3-C2-N2-C7
5	D	482	SIA	C4-C5-N5-C10
5	E	582	SIA	C6-C5-N5-C10
5	F	682	SIA	C6-C7-C8-C9
5	F	682	SIA	O1A-C1-C2-O6
4	B	279	NAG	C3-C2-N2-C7
4	D	479	NAG	C3-C2-N2-C7

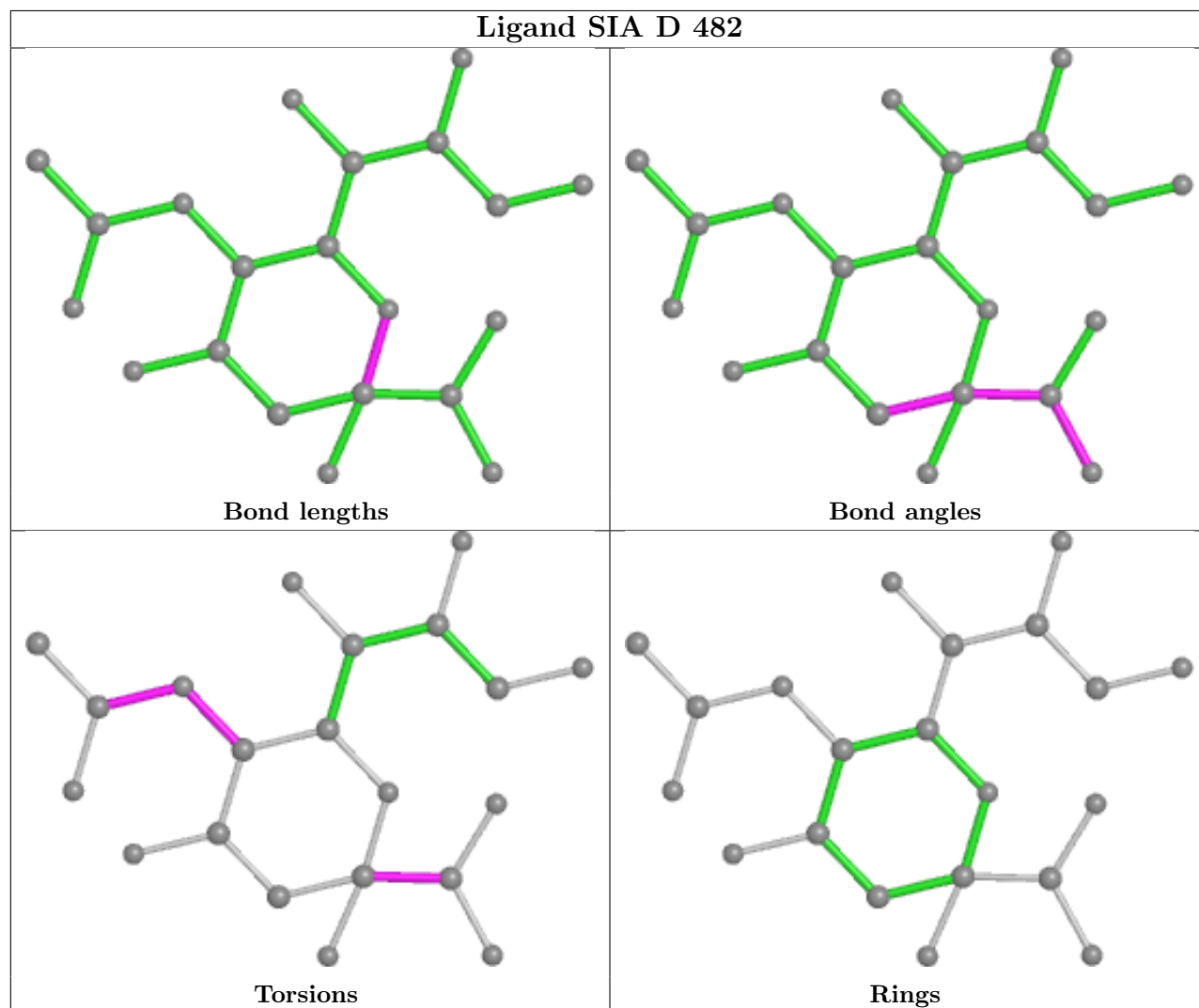
There are no ring outliers.

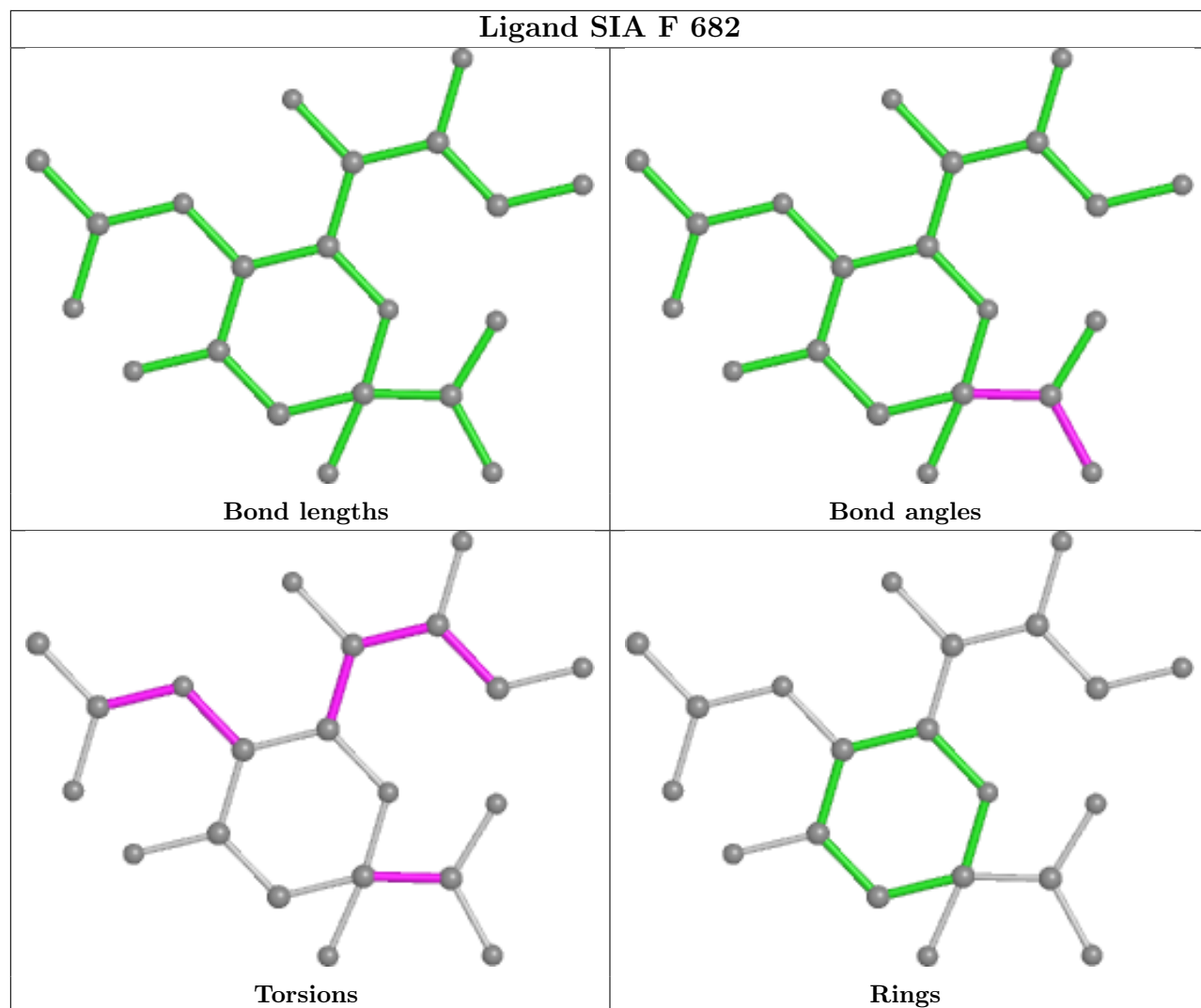
11 monomers are involved in 37 short contacts:

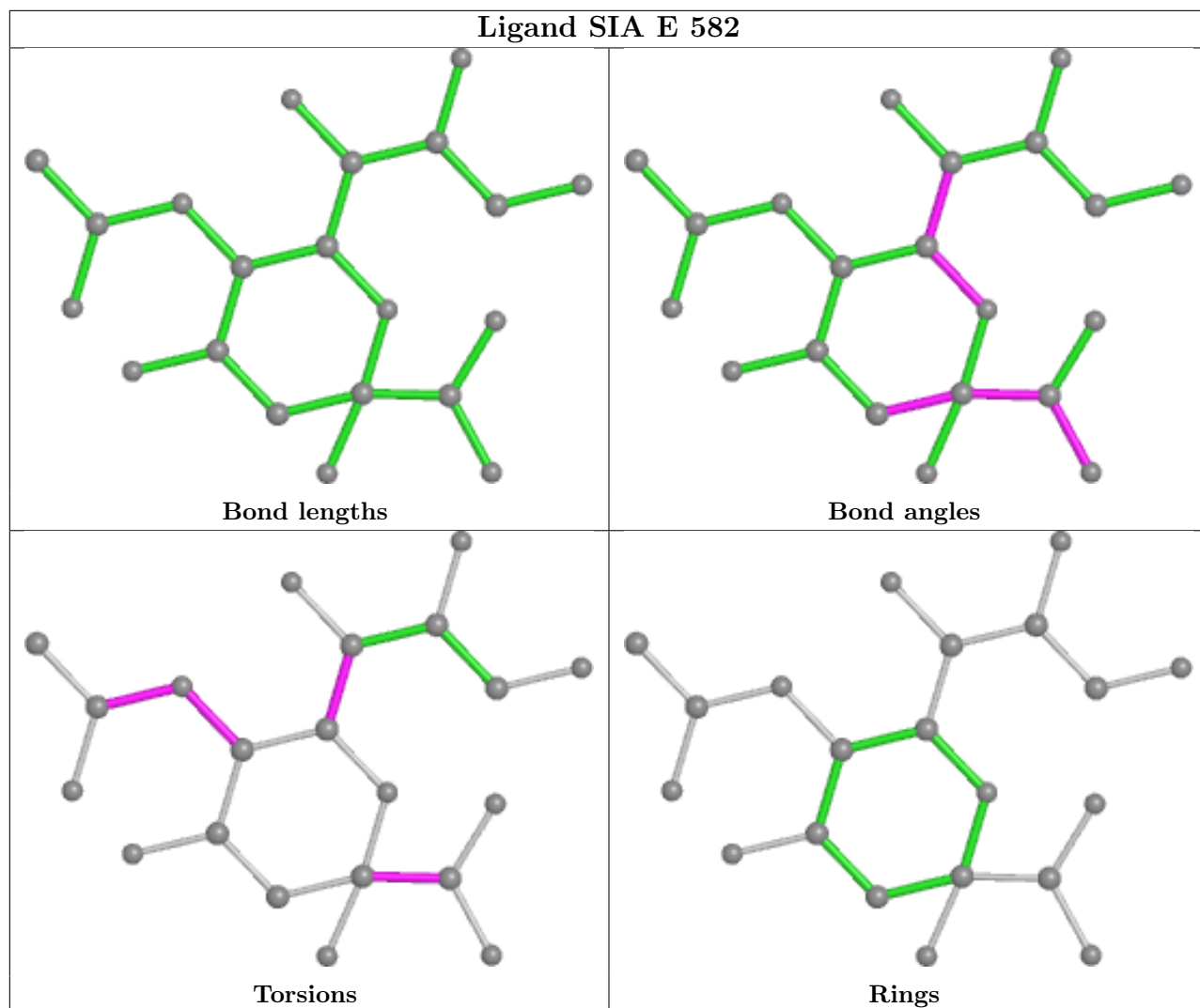
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	679	NAG	2	0
6	C	184	SO4	1	0
5	D	482	SIA	2	0
3	E	1	GD7	2	0
5	F	682	SIA	4	0
4	A	179	NAG	5	0
5	E	582	SIA	6	0
5	A	182	SIA	6	0
5	C	382	SIA	5	0
4	E	579	NAG	1	0
5	B	282	SIA	5	0

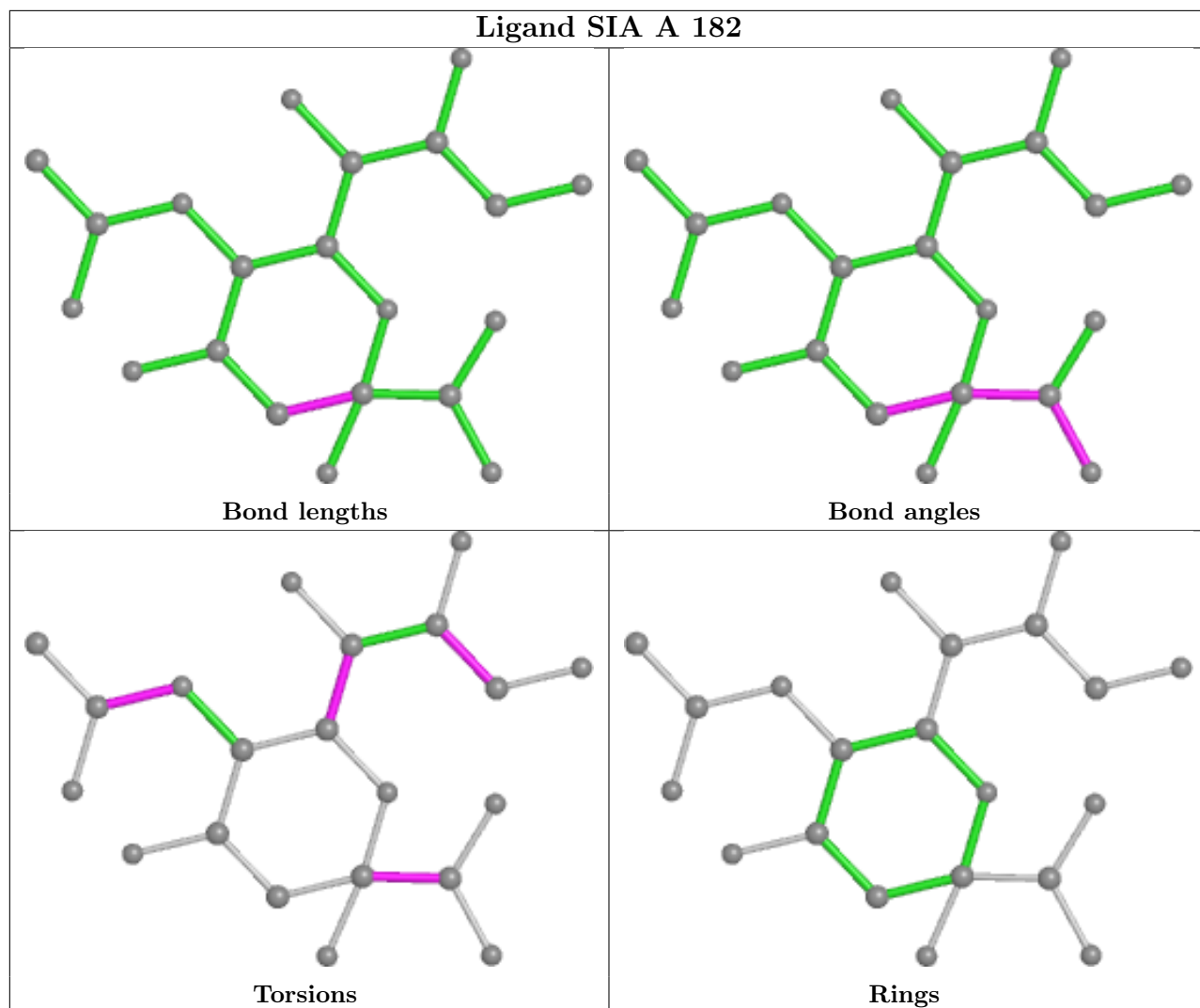
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

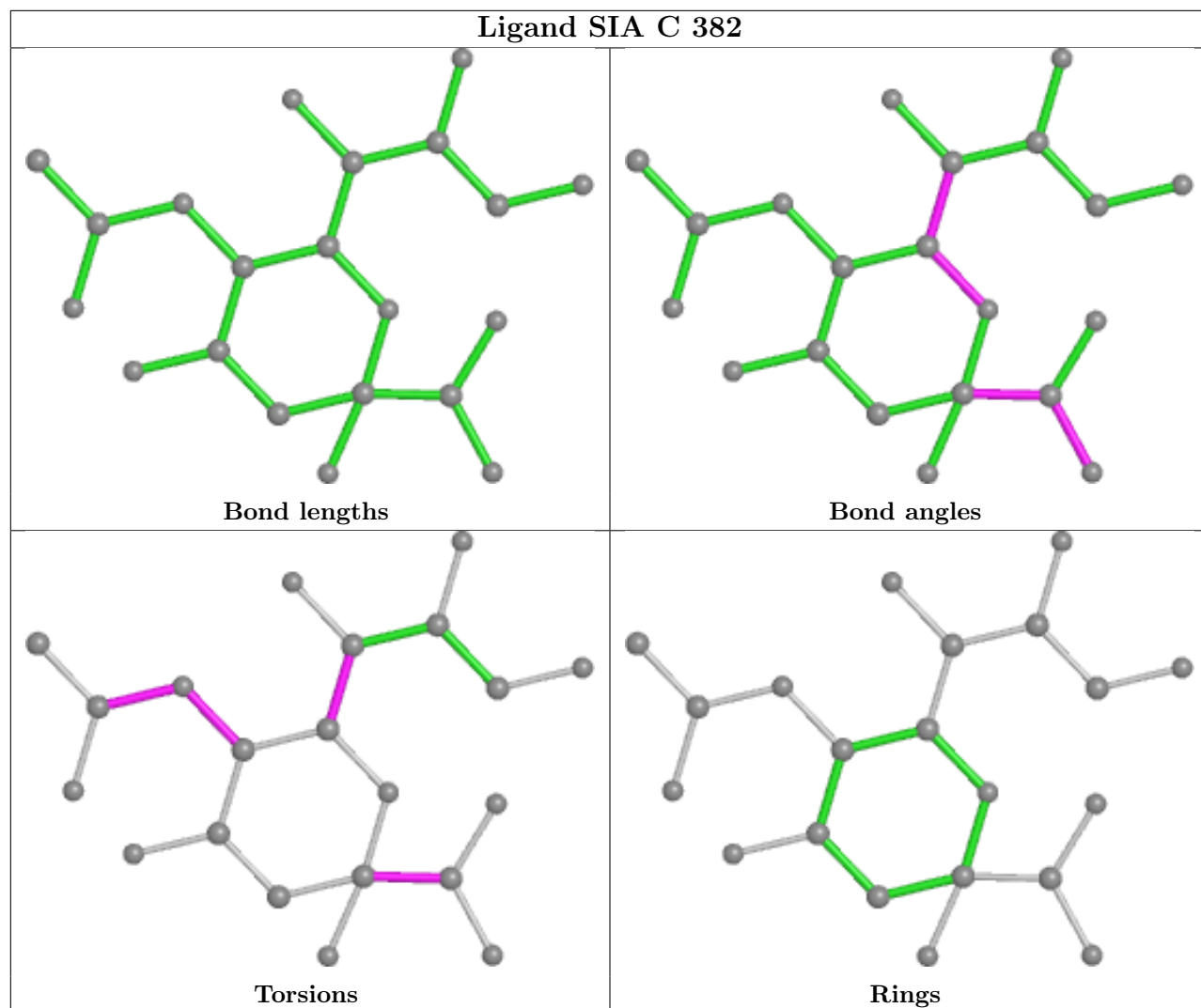
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

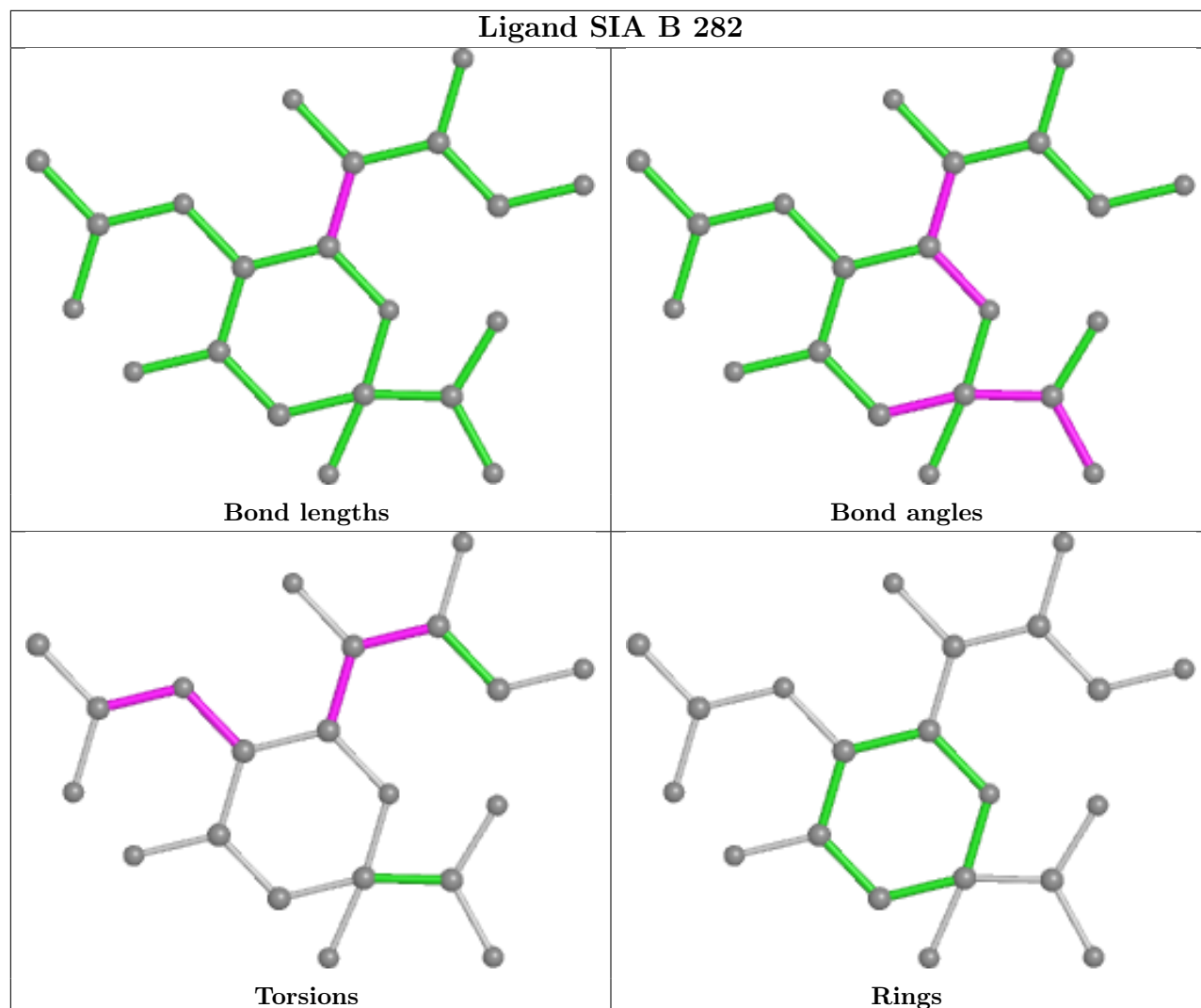












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	532/532 (100%)	-0.21	7 (1%) 77 78	10, 27, 69, 89	0
1	B	531/532 (99%)	-0.21	4 (0%) 86 87	12, 32, 68, 90	0
1	C	531/532 (99%)	-0.35	4 (0%) 86 87	6, 24, 46, 83	0
1	D	532/532 (100%)	-0.21	9 (1%) 70 72	9, 27, 69, 89	0
1	E	531/532 (99%)	-0.19	2 (0%) 92 93	11, 31, 69, 88	0
1	F	531/532 (99%)	-0.34	4 (0%) 86 87	8, 25, 46, 92	0
All	All	3188/3192 (99%)	-0.25	30 (0%) 84 85	6, 27, 64, 92	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1342	HIS	6.3
1	B	2340	ASN	5.2
1	D	4341	PHE	5.0
1	D	4340	ASN	4.6
1	A	1341	PHE	4.6
1	A	1340	ASN	4.6
1	E	5340	ASN	4.4
1	D	4342	HIS	4.4
1	F	6341	PHE	4.3
1	F	6342	HIS	4.3
1	F	6340	ASN	3.7
1	D	4317	PRO	3.3
1	D	4307	ASP	3.1
1	F	6339	ARG	2.8
1	E	5342	HIS	2.7
1	D	4376	LYS	2.5
1	B	2341	PHE	2.5
1	D	4318	LEU	2.5
1	B	2404	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	3341	PHE	2.4
1	A	1450	GLN	2.4
1	C	3340	ASN	2.4
1	B	2406	GLY	2.4
1	A	1317	PRO	2.3
1	C	3108	ILE	2.3
1	D	4314	GLU	2.2
1	A	1021	SER	2.2
1	C	3342	HIS	2.1
1	A	1401	GLU	2.1
1	D	4399	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

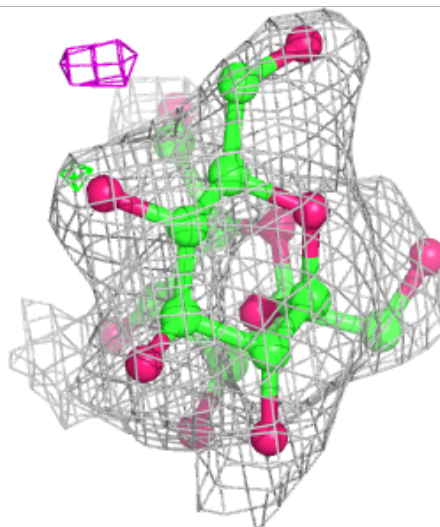
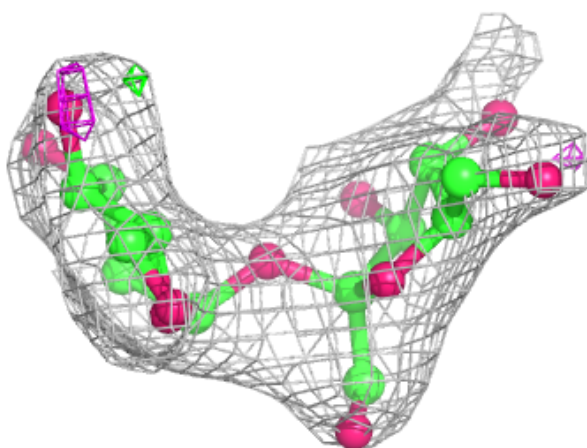
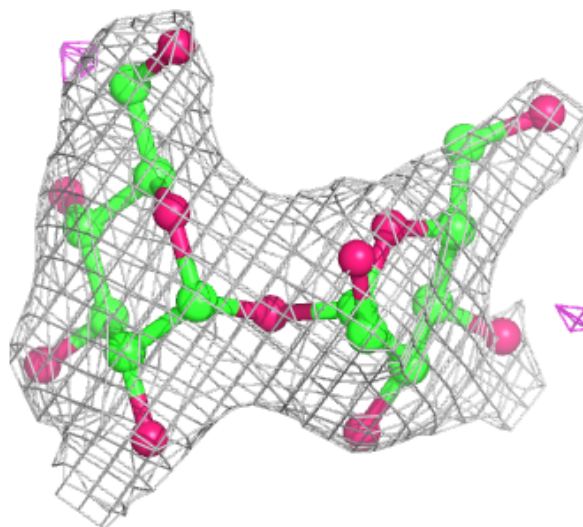
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	FRU	J	2	12/12	0.83	0.25	69,70,73,77	0
2	GLC	K	1	11/12	0.90	0.16	66,68,68,69	0
2	FRU	K	2	12/12	0.90	0.18	67,70,72,73	0
2	FRU	G	2	12/12	0.91	0.19	66,70,71,71	0
2	GLC	J	1	11/12	0.92	0.17	61,62,63,65	0
2	GLC	G	1	11/12	0.92	0.18	57,60,61,62	0
2	GLC	H	1	11/12	0.92	0.17	63,65,65,66	0
2	FRU	H	2	12/12	0.92	0.16	63,65,66,67	0
2	FRU	L	2	12/12	0.92	0.16	31,34,36,39	0
2	GLC	L	1	11/12	0.96	0.14	27,30,31,33	0
2	GLC	I	1	11/12	0.96	0.16	27,28,29,31	0
2	FRU	I	2	12/12	0.97	0.13	28,33,34,38	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.

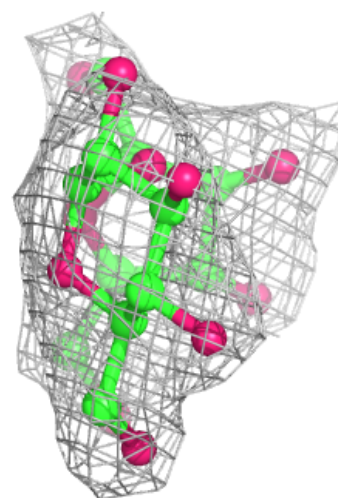
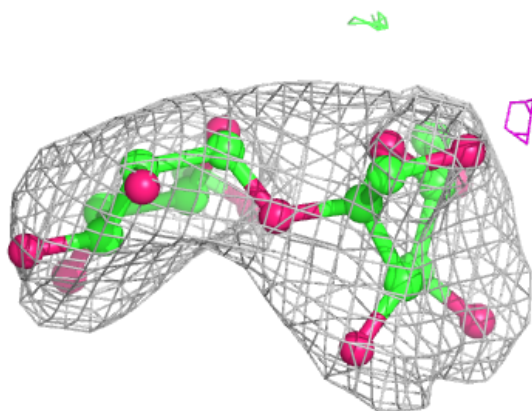
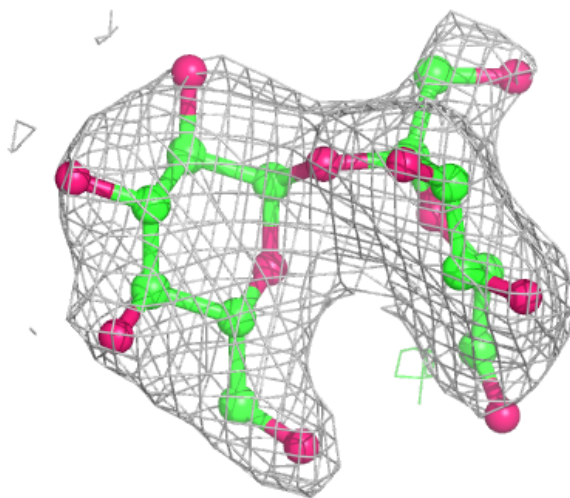
**Electron density around Chain G:**

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



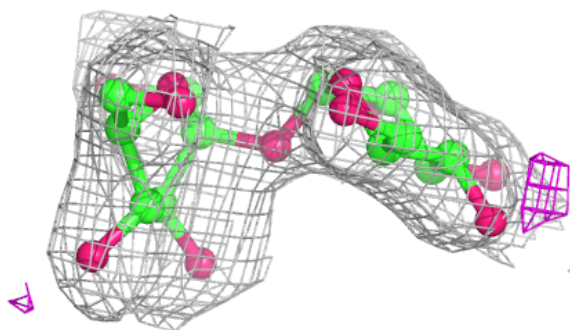
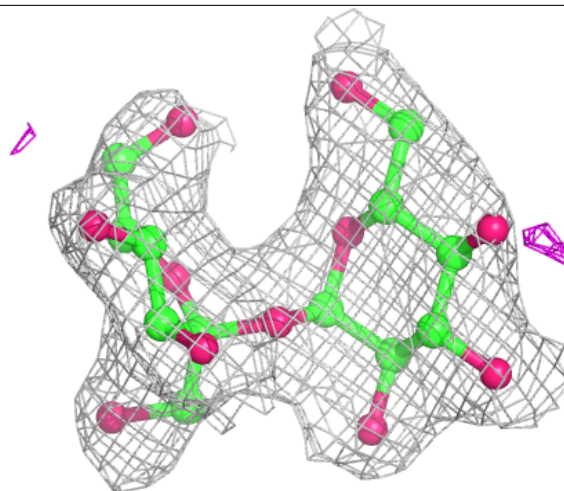
**Electron density around Chain H:**

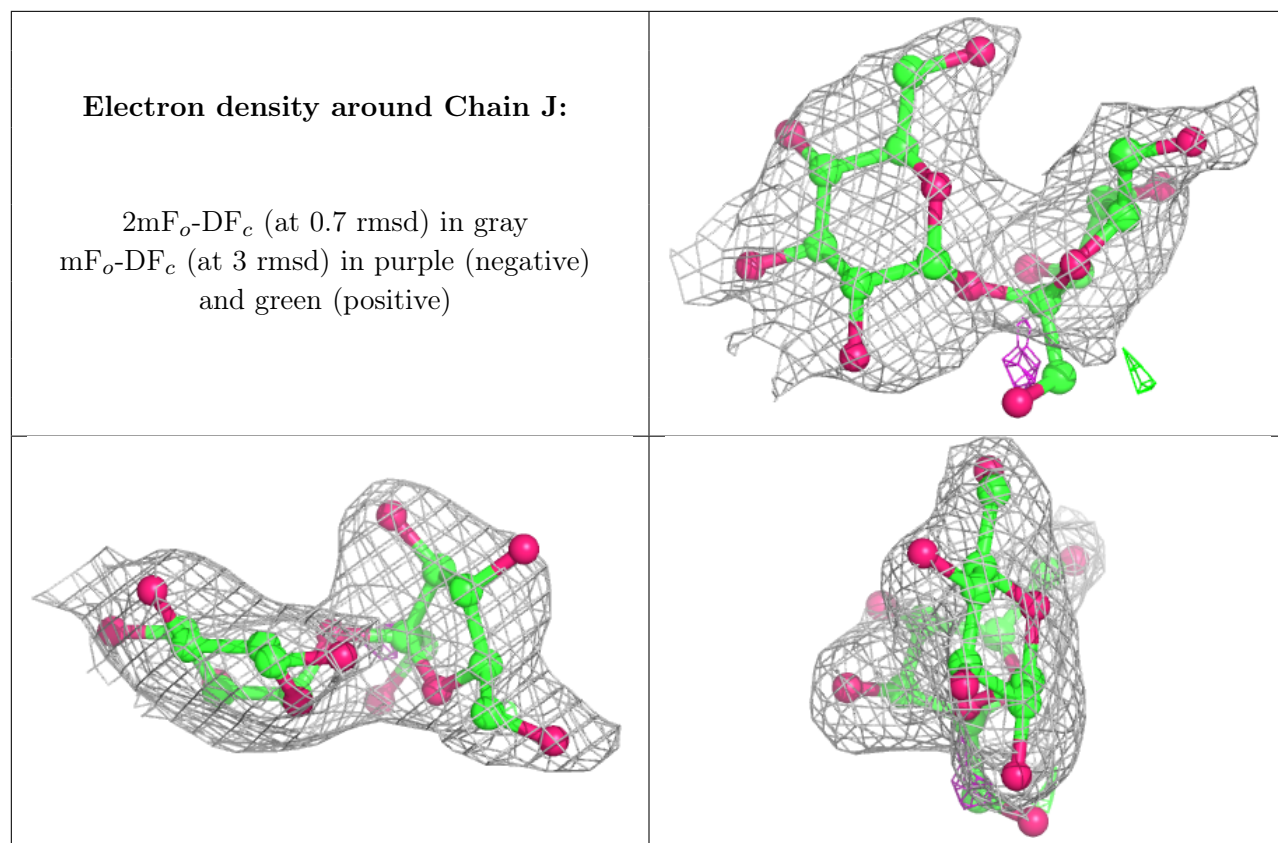
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain I:**

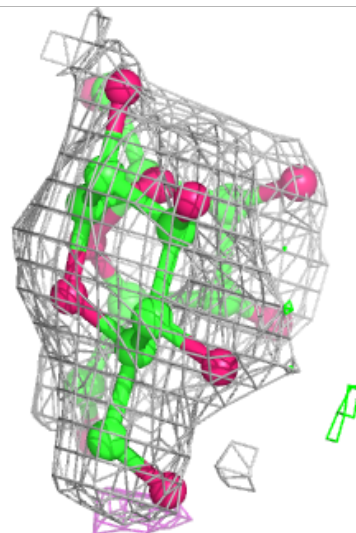
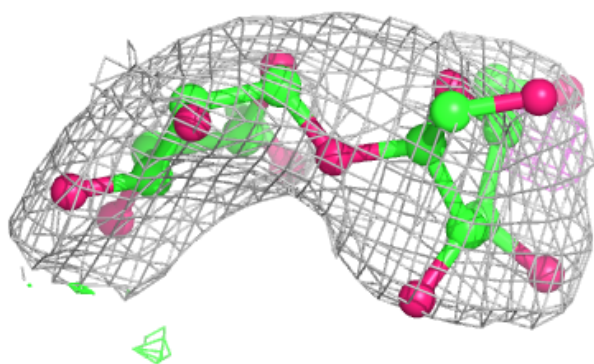
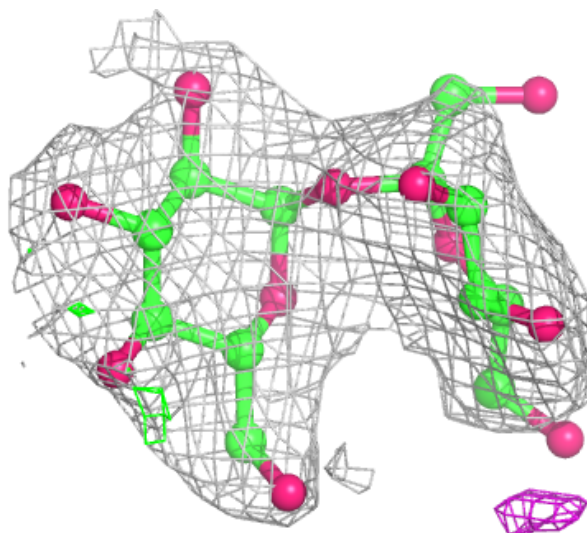
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

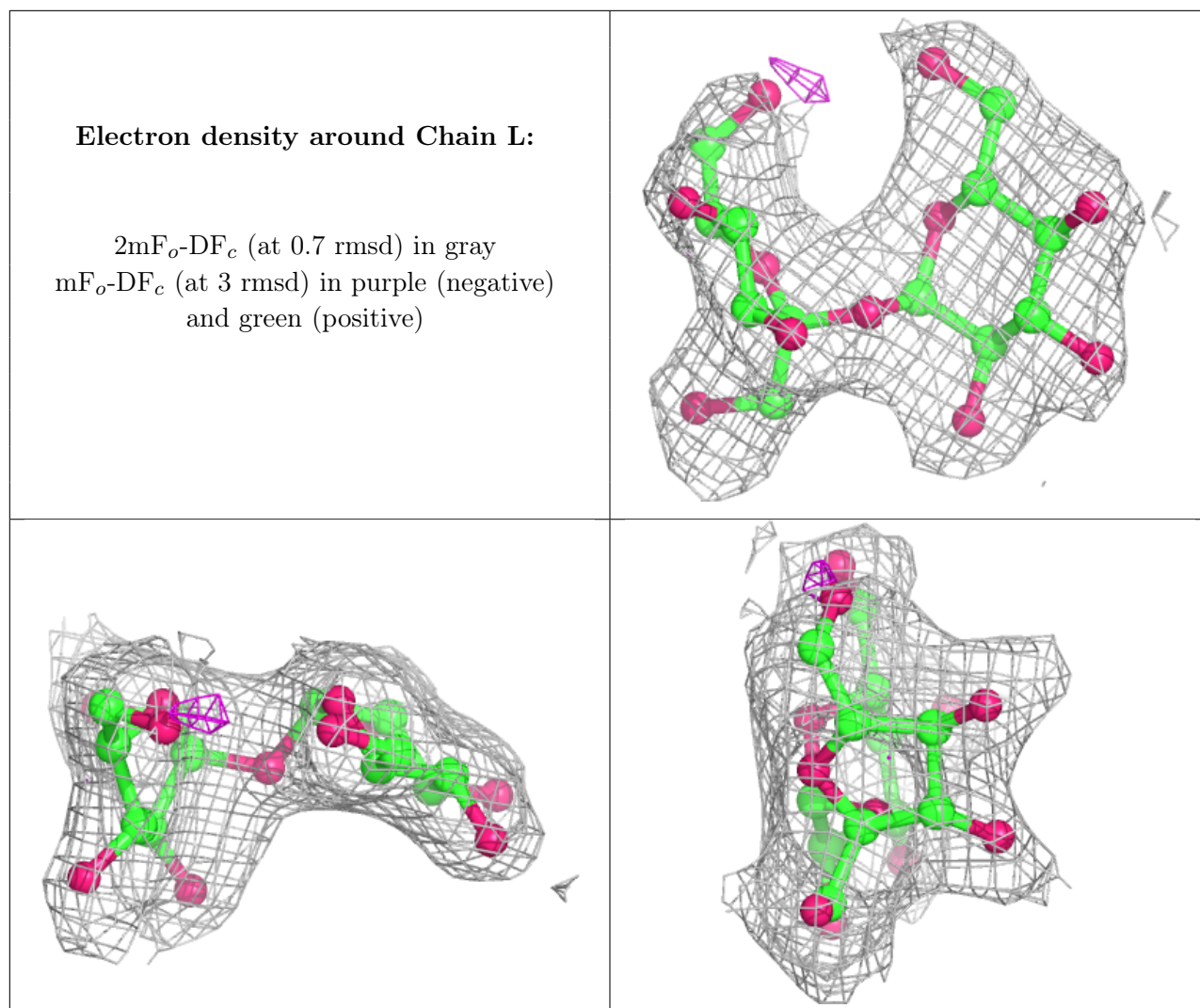




**Electron density around Chain K:**

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





## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	NAG	A	179	14/15	0.61	0.36	59,62,64,64	0
5	SIA	D	482	21/21	0.61	0.41	90,97,100,100	0
4	NAG	C	379	14/15	0.66	0.40	68,73,75,75	0
6	SO4	F	685	5/5	0.66	0.54	130,131,131,131	0
5	SIA	A	182	21/21	0.71	0.38	80,90,91,92	0
6	SO4	F	684	5/5	0.76	0.37	105,106,106,106	0
4	NAG	D	479	14/15	0.76	0.35	59,62,65,65	0
4	NAG	F	679	14/15	0.78	0.33	64,69,70,71	0

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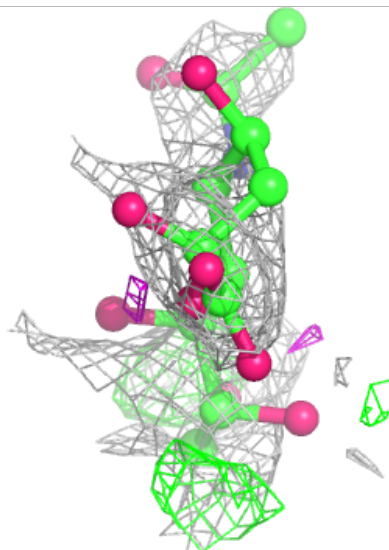
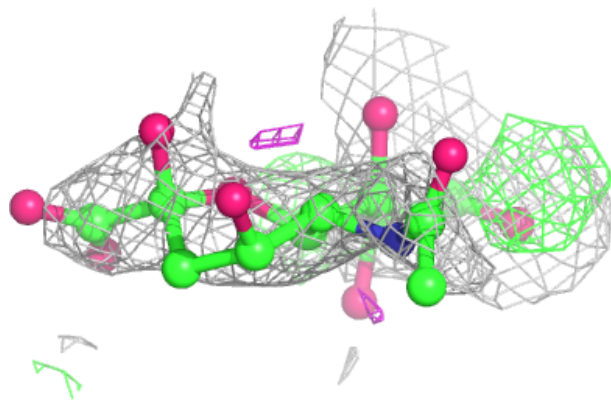
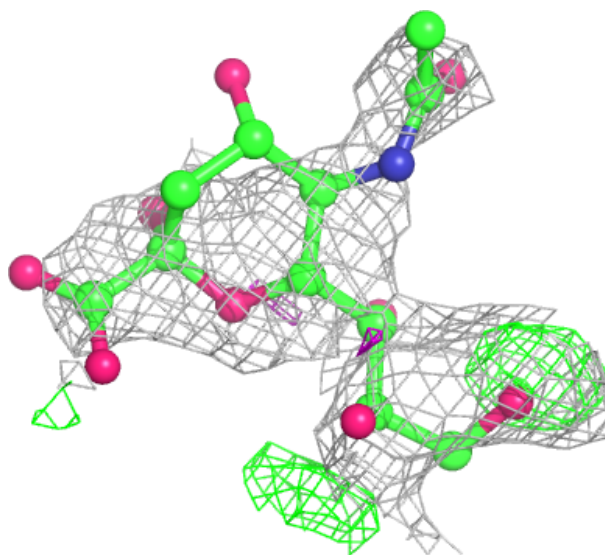
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	SO4	B	385	5/5	0.79	0.35	109,110,110,111	0
5	SIA	C	382	21/21	0.79	0.28	67,78,82,82	0
5	SIA	E	582	21/21	0.79	0.30	36,54,60,61	0
5	SIA	B	282	21/21	0.80	0.32	46,59,64,65	0
6	SO4	C	184	5/5	0.81	0.42	122,122,122,123	0
6	SO4	D	585	5/5	0.82	0.43	120,121,121,121	0
4	NAG	E	579	14/15	0.83	0.34	63,68,71,71	0
4	NAG	B	279	14/15	0.83	0.47	69,73,77,77	0
5	SIA	F	682	21/21	0.84	0.26	58,65,68,68	0
6	SO4	A	284	5/5	0.85	0.38	125,125,125,125	0
6	SO4	A	185	5/5	0.85	0.49	133,133,134,134	0
6	SO4	D	484	5/5	0.86	0.38	128,128,128,129	0
6	SO4	C	384	5/5	0.86	0.24	99,100,100,100	0
6	SO4	E	584	5/5	0.88	0.24	96,96,96,97	0
6	SO4	F	485	5/5	0.89	0.33	115,115,115,115	0
6	SO4	B	285	5/5	0.90	0.27	91,92,92,93	0
3	GD7	D	1	10/10	0.91	0.27	44,49,51,53	0
3	GD7	A	1	10/10	0.92	0.30	45,50,53,55	0
3	GD7	B	1	10/10	0.94	0.25	39,43,44,45	0
3	GD7	F	1	10/10	0.95	0.27	34,41,41,42	0
3	GD7	E	1	10/10	0.96	0.23	33,40,43,44	0
3	GD7	C	1	10/10	0.96	0.28	39,44,45,45	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.



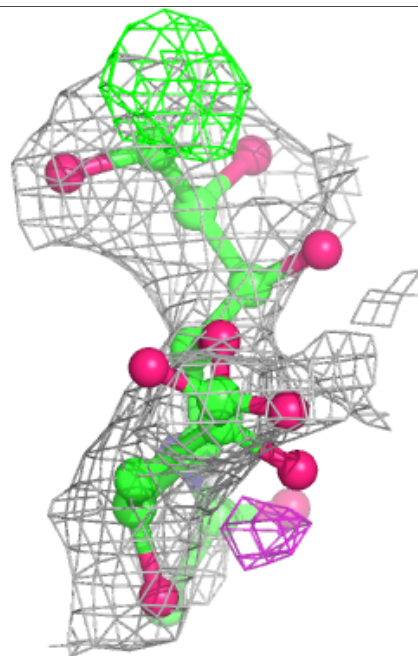
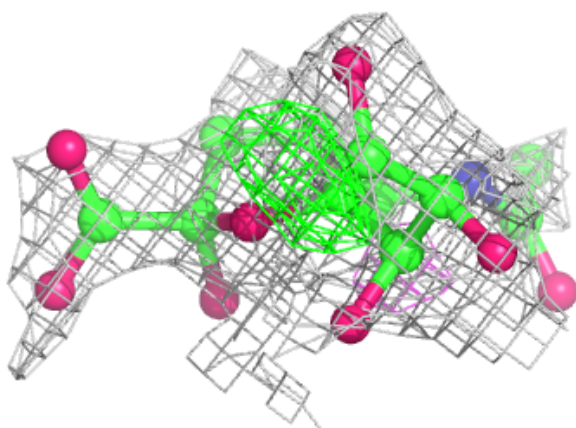
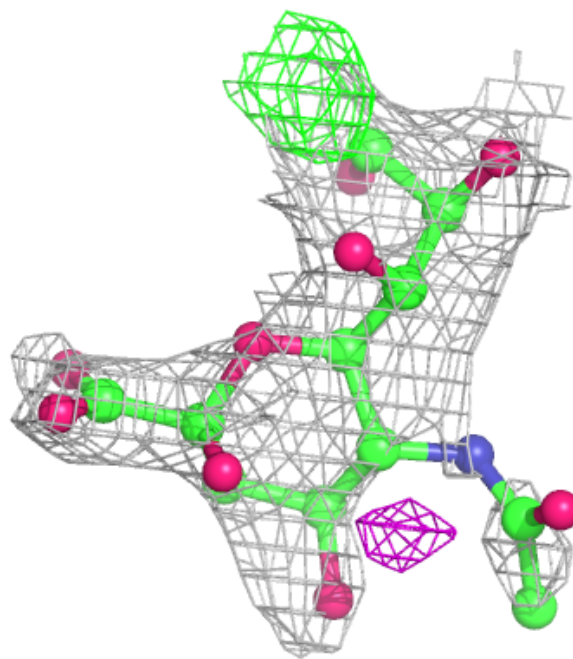
**Electron density around SIA D 482:**

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



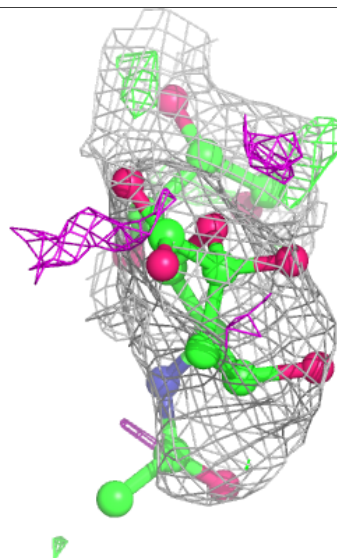
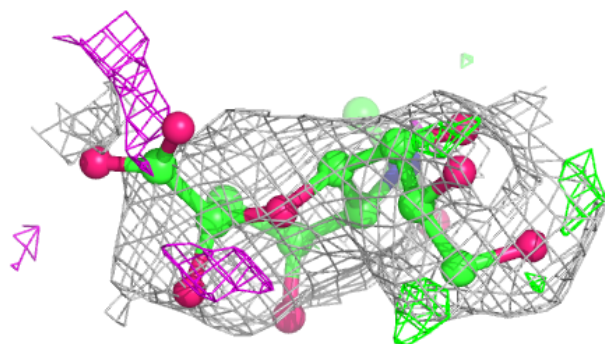
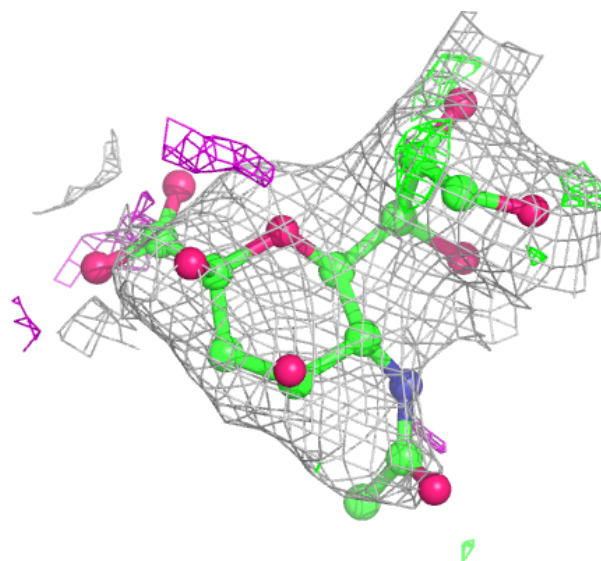
**Electron density around SIA A 182:**

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



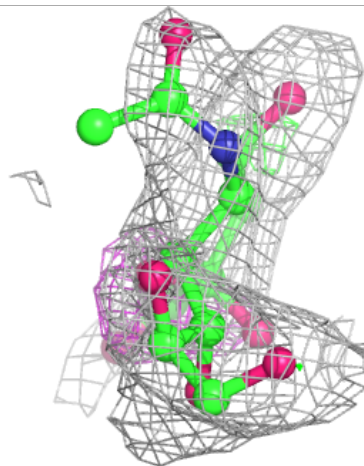
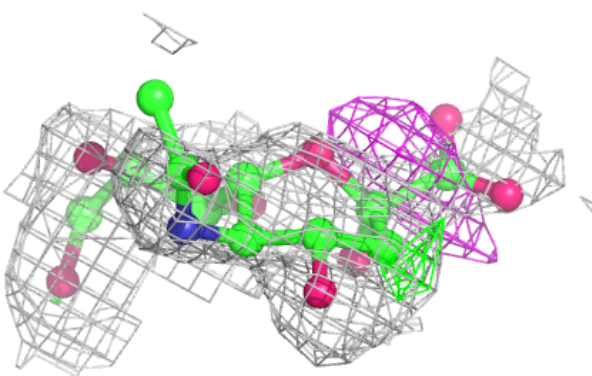
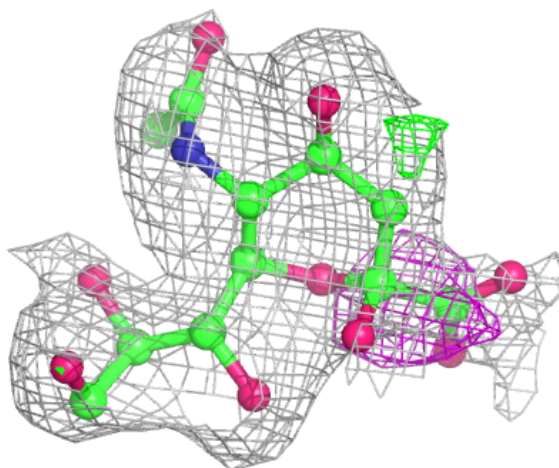
**Electron density around SIA C 382:**

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



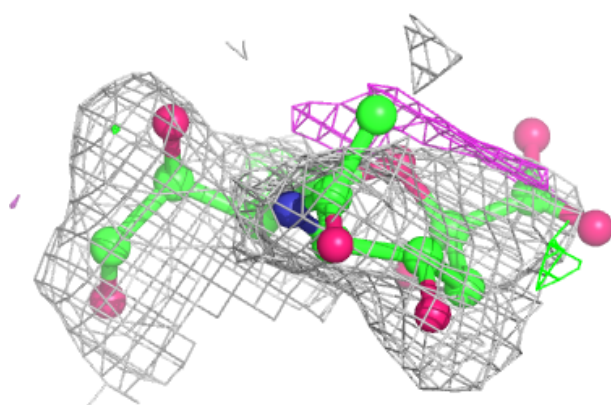
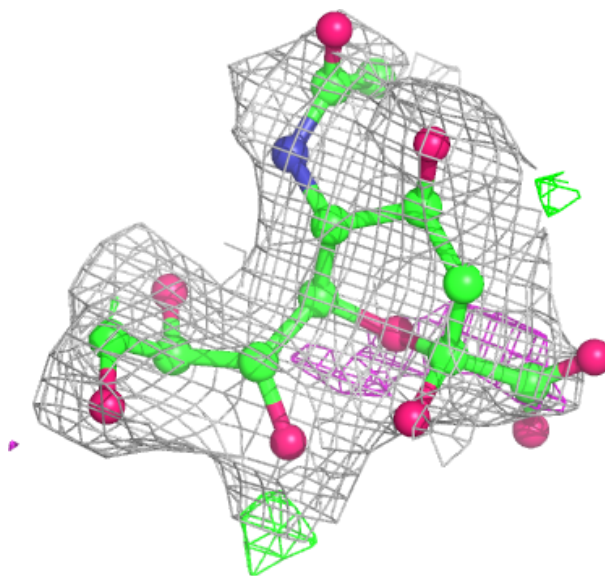
**Electron density around SIA E 582:**

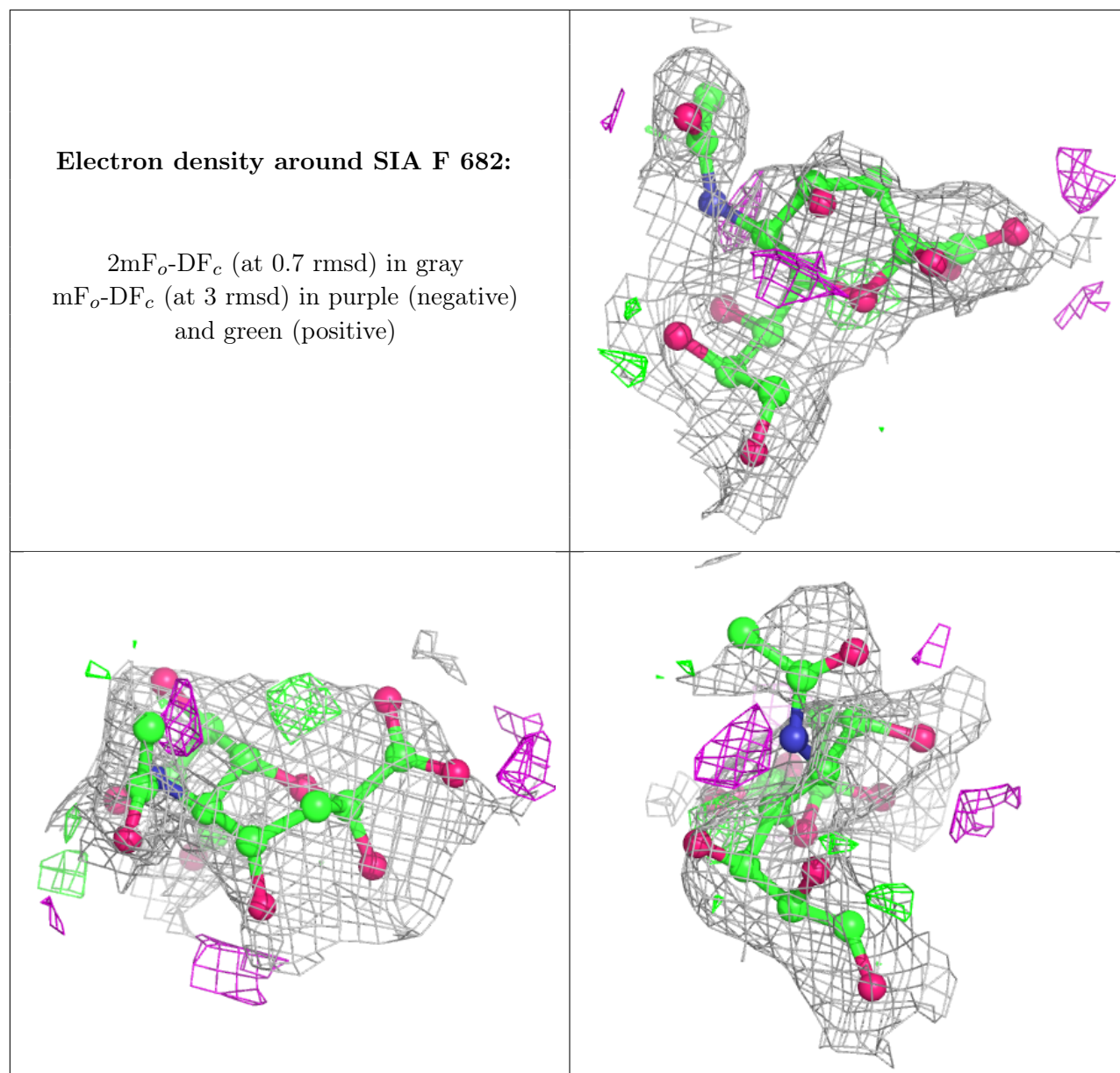
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around SIA B 282:**

$2mF_o-DF_c$  (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.