



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 06:33 PM EDT

PDB ID : 2OYH
Title : Crystal Structure of Fragment D of gammaD298,301A Fibrinogen with the Peptide Ligand Gly-His-Arg-Pro-Amide
Authors : Kostelansky, M.S.; Gorkun, O.V.; Lord, S.T.
Deposited on : 2007-02-22
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
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) : 2.23.2

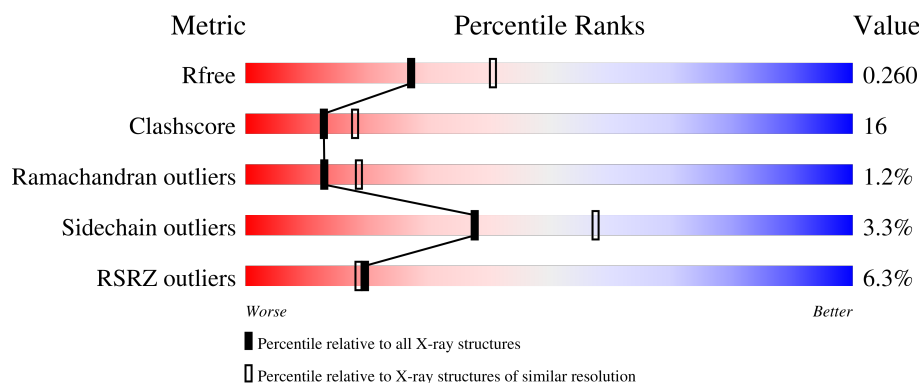
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	66	<div> <div>12%</div> <div> <div></div> <div>52%</div> <div>44%</div> <div>• •</div> </div> </div>
1	D	66	<div> <div>32%</div> <div> <div></div> <div>48%</div> <div>32%</div> <div>•</div> <div>18%</div> </div> </div>
2	B	313	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>32%</div> <div>•</div> <div>5%</div> </div> </div>
2	E	313	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>21%</div> <div>•</div> <div>6%</div> </div> </div>
3	C	311	<div> <div>5%</div> <div> <div></div> <div>71%</div> <div>22%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	F	311	
4	G	4	
4	H	4	
4	I	4	
4	J	4	
5	K	3	
5	L	3	

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	NAG	K	2	-	-	-	X
5	NAG	L	1	-	-	X	-
5	FUC	L	3	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10847 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 Fibrinogen alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	64	Total	C	N	O	S	0	0	0
			523	322	99	99	3			
1	D	54	Total	C	N	O	S	0	0	0
			442	270	84	85	3			

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	298	Total	C	N	O	S	0	0	0
			2392	1494	422	454	22			
2	E	295	Total	C	N	O	S	0	0	0
			2369	1480	418	449	22			

- Molecule 3 is a protein called Fibrinogen gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	299	Total	C	N	O	S	0	0	0
			2393	1521	403	458	11			
3	F	285	Total	C	N	O	S	0	0	0
			2277	1448	384	434	11			

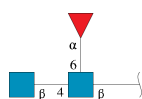
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	298	ALA	ASP	engineered mutation	UNP P02679
C	301	ALA	ASP	engineered mutation	UNP P02679
F	298	ALA	ASP	engineered mutation	UNP P02679
F	301	ALA	ASP	engineered mutation	UNP P02679

- Molecule 4 is a protein called GHRP peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			33	19	9	5			
4	H	4	Total	C	N	O	0	0	0
			33	19	9	5			
4	I	4	Total	C	N	O	0	0	0
			33	19	9	5			
4	J	4	Total	C	N	O	0	0	0
			33	19	9	5			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	K	3	Total	C	N	O	0	0	0
			38	22	2	14			
5	L	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		
6	C	1	Total	Ca	0	0
			1	1		
6	E	1	Total	Ca	0	0
			1	1		
6	F	1	Total	Ca	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	9	Total	O	0	0
			9	9		
7	B	54	Total	O	0	0
			54	54		
7	C	29	Total	O	0	0
			29	29		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	11	Total 11	O 11	0	0
7	E	91	Total 91	O 91	0	0
7	F	44	Total 44	O 44	0	0
7	J	1	Total 1	O 1	0	0

3 Residue-property plots [i](#)

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

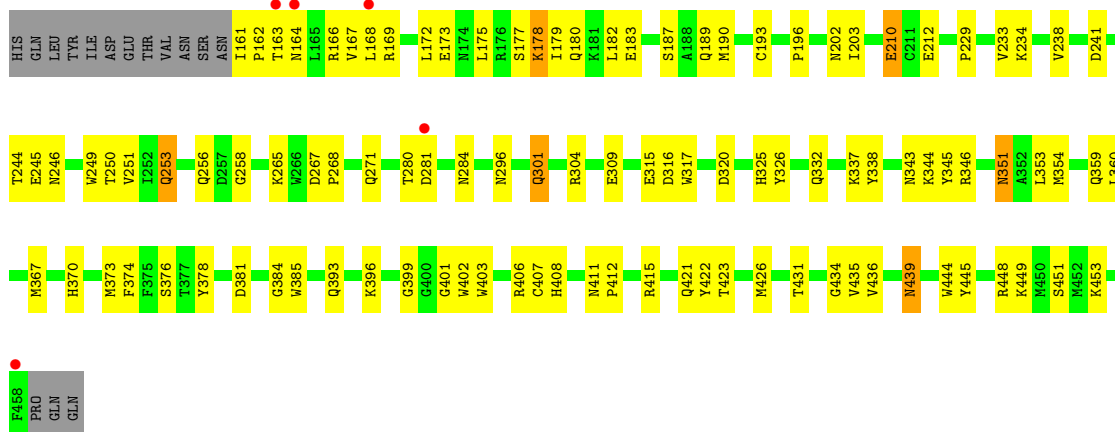
- Molecule 1: Fibrinogen alpha chain



- Molecule 1: Fibrinogen alpha chain

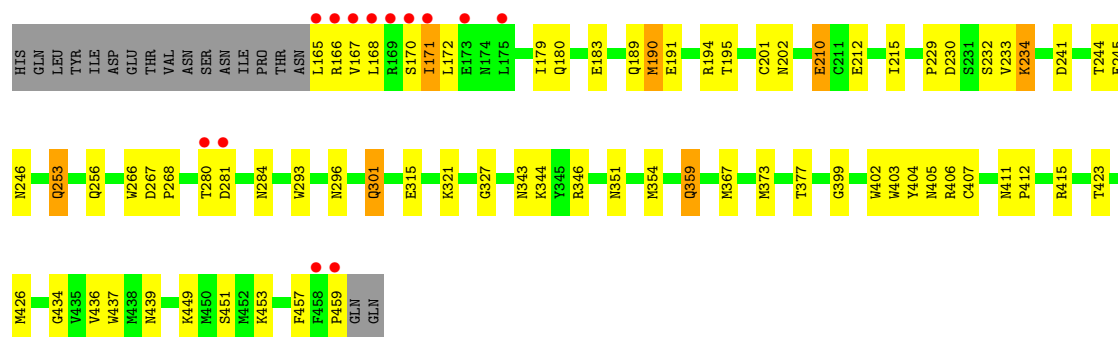


- Molecule 2: Fibrinogen beta chain



- Molecule 2: Fibrinogen beta chain

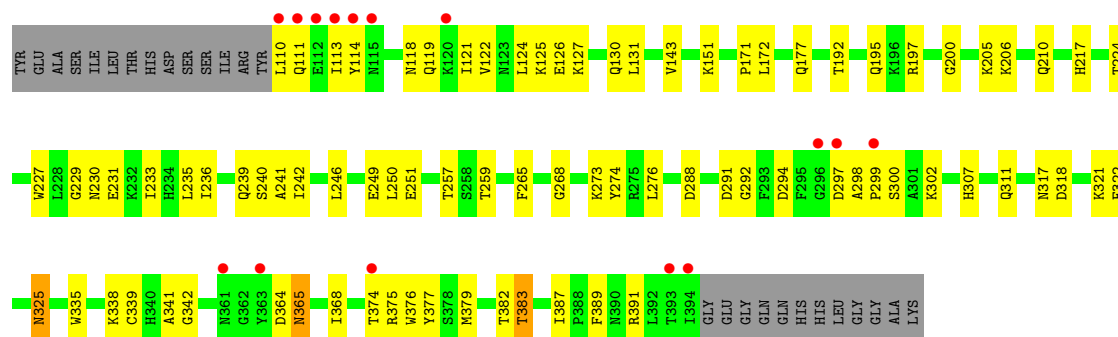




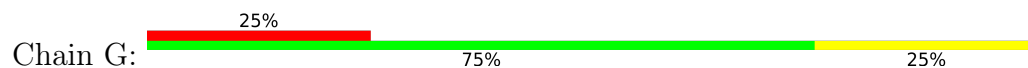
• Molecule 3: Fibrinogen gamma chain



• Molecule 3: Fibrinogen gamma chain



• Molecule 4: GHRP peptide



• Molecule 4: GHRP peptide



G1
H2
R3
P4

- Molecule 4: GHRP peptide



G1
H2
R3
P4

- Molecule 4: GHRP peptide



G1
H2
R3
P4

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



MAG1
MAG2
FUC3

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



MAG1
MAG2
FUC3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.16Å 94.12Å 226.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 2.40 43.46 – 2.41	Depositor EDS
% Data completeness (in resolution range)	95.5 (18.00-2.40) 95.6 (43.46-2.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 2.39Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.220 , 0.259 0.221 , 0.260	Depositor DCC
R_{free} test set	3604 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10847	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.94% 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: FUC, CA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/524	0.51	0/699
1	D	0.29	0/442	0.51	0/588
2	B	0.35	0/2453	0.60	0/3312
2	E	0.38	0/2430	0.65	1/3280 (0.0%)
3	C	0.34	0/2459	0.54	0/3327
3	F	0.36	0/2340	0.60	0/3165
4	G	0.48	0/34	0.46	0/43
4	H	0.46	0/34	0.49	0/43
4	I	0.47	0/34	0.44	0/43
4	J	0.54	0/34	0.53	0/43
All	All	0.36	0/10784	0.59	1/14543 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	399	GLY	N-CA-C	6.85	130.23	113.10

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	523	0	547	36	0
1	D	442	0	460	27	0
2	B	2392	0	2262	93	0
2	E	2369	0	2238	73	0
3	C	2393	0	2248	62	0
3	F	2277	0	2140	76	0
4	G	33	0	32	1	0
4	H	33	0	32	3	0
4	I	33	0	32	3	0
4	J	33	0	32	1	0
5	K	38	0	34	2	0
5	L	38	0	34	9	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
7	A	9	0	0	0	0
7	B	54	0	0	3	0
7	C	29	0	0	1	0
7	D	11	0	0	0	0
7	E	91	0	0	1	0
7	F	44	0	0	1	0
7	J	1	0	0	0	0
All	All	10847	0	10091	341	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 16.

All (341) 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)
3:F:374:THR:HG22	3:F:376:TRP:H	1.23	1.02
3:C:148:ILE:H	3:C:148:ILE:HD12	1.33	0.92
2:E:234:LYS:H	2:E:234:LYS:HD2	1.33	0.92
1:A:128:GLU:HG2	1:A:129:LYS:H	1.35	0.90
3:C:249:GLU:HB2	3:C:383:THR:HG23	1.51	0.90
3:F:151:LYS:HB3	3:F:239:GLN:HE22	1.37	0.88
1:A:127:ILE:HG22	1:A:130:VAL:HG23	1.55	0.86
1:D:185:LEU:HD23	2:E:171:ILE:HD11	1.61	0.83
2:E:373:MET:HE1	2:E:405:ASN:HA	1.60	0.82
3:F:307:HIS:HE1	3:F:341:ALA:H	1.27	0.81
1:A:130:VAL:O	1:A:134:GLN:HG3	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:LEU:HD11	3:F:111:GLN:HB2	1.62	0.80
3:F:197:ARG:HB2	3:F:382:THR:HB	1.64	0.79
2:B:367:MET:SD	2:B:406:ARG:HD3	2.22	0.79
2:E:423:THR:N	2:E:426:MET:HE3	1.98	0.79
1:A:135:LEU:HG	1:A:139:ASN:HD21	1.46	0.79
5:L:1:NAG:H61	5:L:3:FUC:H3	1.66	0.78
2:E:165:LEU:HD11	2:E:168:LEU:HD22	1.64	0.77
3:F:249:GLU:HB2	3:F:383:THR:HG23	1.67	0.76
2:B:316:ASP:HB2	2:B:445:TYR:OH	1.86	0.76
3:C:151:LYS:HB3	3:C:239:GLN:HE22	1.51	0.76
2:B:202:ASN:HD22	2:B:284:ASN:HD22	1.31	0.75
2:B:423:THR:N	2:B:426:MET:HE3	2.01	0.75
1:D:136:LEU:HD21	3:F:111:GLN:HG3	1.68	0.75
2:B:163:THR:HB	2:B:166:ARG:HD2	1.69	0.74
4:H:2:HIS:CD2	4:H:4:PRO:HD3	2.22	0.74
1:A:127:ILE:HG12	1:A:128:GLU:H	1.53	0.73
3:C:108:ARG:O	3:C:112:GLU:HG3	1.88	0.73
2:B:439:ASN:H	2:B:439:ASN:HD22	1.37	0.73
2:E:439:ASN:HD22	2:E:439:ASN:H	1.38	0.72
1:A:153:ASP:O	1:A:157:LYS:HG2	1.88	0.72
2:E:359:GLN:H	2:E:359:GLN:HE21	1.36	0.71
2:E:230:ASP:HB3	2:E:233:VAL:HG12	1.72	0.71
5:L:1:NAG:H61	5:L:3:FUC:H5	1.72	0.71
1:A:127:ILE:HG22	1:A:130:VAL:CG2	2.21	0.70
1:D:166:SER:HB3	2:E:195:THR:HG22	1.73	0.70
3:F:307:HIS:CE1	3:F:341:ALA:H	2.08	0.70
5:L:1:NAG:H62	5:L:2:NAG:H2	1.72	0.70
2:B:423:THR:H	2:B:426:MET:HE3	1.54	0.69
2:B:351:ASN:HD21	2:B:354:MET:H	1.40	0.69
1:D:144:LEU:HD21	1:D:182:GLN:HG2	1.75	0.69
2:E:234:LYS:H	2:E:234:LYS:CD	2.06	0.68
2:E:415:ARG:O	2:E:434:GLY:HA2	1.93	0.68
3:F:200:GLY:HA2	7:F:409:HOH:O	1.93	0.68
2:E:373:MET:CE	2:E:405:ASN:HA	2.23	0.68
1:D:139:ASN:HB3	3:F:114:TYR:CZ	2.30	0.67
2:B:351:ASN:ND2	2:B:354:MET:H	1.93	0.66
2:B:202:ASN:ND2	2:B:284:ASN:HB2	2.10	0.66
3:F:276:LEU:HD23	3:F:276:LEU:C	2.15	0.66
2:E:202:ASN:HD22	2:E:284:ASN:HD22	1.42	0.66
1:A:128:GLU:HG2	1:A:129:LYS:N	2.08	0.66
3:C:307:HIS:HE1	3:C:341:ALA:H	1.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:251:GLU:HB3	3:C:381:LYS:HB2	1.78	0.65
3:C:252:ASP:OD2	3:C:256:ARG:HB2	1.95	0.65
1:A:182:GLN:O	1:A:186:GLU:HG2	1.96	0.65
1:A:168:ALA:HA	2:B:189:GLN:HE22	1.62	0.65
2:B:351:ASN:OD1	2:B:354:MET:HB2	1.96	0.65
2:B:367:MET:HB2	2:B:406:ARG:HB3	1.78	0.65
5:L:1:NAG:H4	5:L:2:NAG:N2	2.10	0.65
3:C:148:ILE:H	3:C:148:ILE:CD1	2.08	0.64
1:A:188:VAL:HG21	2:B:167:VAL:HG21	1.79	0.64
2:B:439:ASN:HD22	2:B:439:ASN:N	1.95	0.64
2:E:202:ASN:ND2	2:E:284:ASN:HB2	2.13	0.64
3:F:338:LYS:N	3:F:339:CYS:HA	2.11	0.64
1:A:185:LEU:HD22	1:A:189:ILE:HD11	1.80	0.63
2:B:415:ARG:O	2:B:434:GLY:HA2	1.98	0.63
3:C:197:ARG:HB2	3:C:382:THR:HB	1.79	0.63
1:D:136:LEU:HD21	3:F:111:GLN:CG	2.28	0.63
1:A:127:ILE:HG23	1:A:128:GLU:N	2.13	0.63
2:E:201:CYS:O	3:F:143:VAL:HG21	1.98	0.62
3:F:249:GLU:HG2	3:F:259:THR:HG22	1.79	0.62
5:L:1:NAG:H61	5:L:3:FUC:C3	2.29	0.62
1:A:178:TYR:O	1:A:182:GLN:HG3	1.99	0.62
1:A:183:LYS:O	1:A:187:GLN:HG3	1.99	0.62
1:A:135:LEU:HG	1:A:139:ASN:ND2	2.13	0.62
2:E:406:ARG:NH1	4:J:3:ARG:O	2.33	0.61
2:B:343:ASN:OD1	2:B:344:LYS:HE2	2.01	0.61
1:D:178:TYR:O	1:D:182:GLN:HG3	2.00	0.61
3:F:118:ASN:O	3:F:122:VAL:HG23	2.00	0.61
1:A:169:LEU:H	2:B:189:GLN:NE2	1.98	0.60
2:B:161:ILE:N	2:B:162:PRO:HD2	2.17	0.60
3:C:307:HIS:CE1	3:C:341:ALA:H	2.20	0.60
1:A:139:ASN:HB3	3:C:114:TYR:CZ	2.37	0.60
2:E:172:LEU:HD23	2:E:172:LEU:O	2.02	0.59
3:C:148:ILE:HD12	3:C:148:ILE:N	2.12	0.59
2:E:168:LEU:HD21	3:F:110:LEU:HB3	1.84	0.59
3:C:325:ASN:C	3:C:325:ASN:HD22	2.07	0.58
1:A:133:ILE:O	1:A:137:GLN:HG3	2.03	0.58
1:D:169:LEU:H	2:E:189:GLN:HE22	1.50	0.58
2:E:423:THR:H	2:E:426:MET:HE3	1.67	0.58
1:A:127:ILE:N	1:A:130:VAL:HB	2.18	0.58
2:E:212:GLU:O	2:E:215:ILE:HG22	2.04	0.58
2:E:253:GLN:NE2	2:E:451:SER:HA	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:195:GLN:OE1	3:F:382:THR:HG22	2.04	0.58
5:K:1:NAG:H4	5:K:2:NAG:HN2	1.69	0.58
3:C:251:GLU:HG3	3:C:257:THR:HG22	1.85	0.58
1:D:185:LEU:HD13	1:D:185:LEU:O	2.03	0.57
2:B:210:GLU:OE1	2:B:212:GLU:HB3	2.03	0.57
1:D:144:LEU:CD2	1:D:182:GLN:HE21	2.17	0.57
2:B:233:VAL:HG12	2:B:234:LYS:N	2.19	0.57
3:F:288:ASP:OD2	3:F:291:ASP:HB2	2.05	0.57
2:E:367:MET:HB2	2:E:406:ARG:HB3	1.85	0.57
2:B:251:VAL:HG22	2:B:453:LYS:HE2	1.87	0.57
1:D:136:LEU:O	1:D:140:VAL:HG22	2.04	0.56
1:A:151:GLU:OE2	2:B:182:LEU:HD21	2.06	0.56
2:B:229:PRO:HB3	2:B:301:GLN:HE22	1.71	0.56
2:B:315:GLU:HB3	2:B:449:LYS:HB2	1.88	0.56
1:D:158:ILE:HG23	2:E:189:GLN:HE21	1.71	0.56
3:F:297:ASP:OD2	4:I:2:HIS:HB3	2.05	0.56
3:F:374:THR:HG22	3:F:376:TRP:N	2.08	0.56
5:L:1:NAG:H61	5:L:3:FUC:C5	2.36	0.56
1:A:127:ILE:HG12	1:A:128:GLU:OE2	2.05	0.56
2:B:253:GLN:NE2	2:B:451:SER:HA	2.21	0.56
3:F:119:GLN:HA	3:F:119:GLN:NE2	2.20	0.56
2:B:316:ASP:OD2	2:B:320:ASP:HB2	2.06	0.56
2:B:326:TYR:CE2	2:B:353:LEU:HD12	2.41	0.55
2:E:373:MET:HE2	2:E:404:TYR:O	2.06	0.55
3:F:389:PHE:C	3:F:391:ARG:H	2.10	0.55
3:C:365:ASN:HD22	3:C:365:ASN:H	1.55	0.54
2:B:337:LYS:HE2	2:B:374:PHE:CD1	2.43	0.54
2:E:172:LEU:HD22	3:F:113:ILE:HD11	1.90	0.54
3:F:297:ASP:HB2	4:I:2:HIS:HD2	1.72	0.54
2:B:345:TYR:CG	2:B:346:ARG:N	2.76	0.54
2:E:359:GLN:H	2:E:359:GLN:NE2	2.03	0.54
3:F:325:ASN:HD22	3:F:325:ASN:C	2.11	0.54
1:D:169:LEU:H	2:E:189:GLN:NE2	2.05	0.54
2:B:265:LYS:O	2:B:268:PRO:HD2	2.08	0.54
3:F:121:ILE:O	3:F:125:LYS:HG3	2.07	0.54
5:L:1:NAG:H4	5:L:2:NAG:HN2	1.73	0.54
1:A:158:ILE:HG23	2:B:189:GLN:HE21	1.72	0.53
2:B:258:GLY:HA2	7:B:462:HOH:O	2.08	0.53
1:A:150:LEU:HD21	3:C:124:LEU:HD23	1.90	0.53
3:C:338:LYS:N	3:C:339:CYS:HA	2.21	0.53
3:F:292:GLY:C	3:F:302:LYS:HD2	2.28	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:307:HIS:HD2	3:F:335:TRP:O	1.91	0.53
1:D:135:LEU:HD13	1:D:135:LEU:O	2.09	0.53
2:E:165:LEU:HG	2:E:165:LEU:O	2.08	0.53
2:E:457:PHE:O	2:E:459:PRO:HD3	2.07	0.53
1:A:169:LEU:H	2:B:189:GLN:HE22	1.54	0.53
3:F:205:LYS:NZ	3:F:205:LYS:HB3	2.23	0.53
2:E:267:ASP:HB3	2:E:268:PRO:HD3	1.91	0.53
2:B:163:THR:HG22	2:B:166:ARG:CZ	2.39	0.53
3:F:365:ASN:HD22	3:F:365:ASN:H	1.55	0.53
3:C:103:HIS:O	3:C:107:ILE:HB	2.09	0.52
1:A:139:ASN:HB3	3:C:114:TYR:CE1	2.44	0.52
2:E:210:GLU:OE1	2:E:212:GLU:HB3	2.09	0.52
3:F:387:ILE:HD11	3:F:391:ARG:HG2	1.92	0.52
3:C:307:HIS:HD2	3:C:335:TRP:O	1.93	0.52
2:B:202:ASN:HD22	2:B:284:ASN:ND2	2.06	0.52
2:E:423:THR:HG23	2:E:426:MET:HE3	1.92	0.52
3:F:251:GLU:HG3	3:F:257:THR:HG22	1.91	0.52
3:C:195:GLN:OE1	3:C:382:THR:HG22	2.09	0.52
3:C:281:PHE:HB2	3:C:288:ASP:OD2	2.10	0.52
1:D:143:GLN:NE2	3:F:118:ASN:OD1	2.43	0.51
3:F:124:LEU:O	3:F:127:LYS:HB3	2.10	0.51
2:B:359:GLN:O	2:B:360:LEU:HD23	2.11	0.51
2:E:315:GLU:HB3	2:E:449:LYS:HB2	1.92	0.51
2:E:179:ILE:O	2:E:183:GLU:HG3	2.10	0.51
2:B:202:ASN:ND2	2:B:284:ASN:HD22	2.05	0.51
1:D:173:VAL:HG12	1:D:175:LEU:HD22	1.93	0.51
2:B:453:LYS:HE3	7:B:469:HOH:O	2.11	0.50
3:F:172:LEU:H	3:F:239:GLN:HE21	1.58	0.50
1:D:174:ASP:OD2	1:D:177:ASP:HB2	2.11	0.50
1:A:185:LEU:HD22	1:A:189:ILE:CD1	2.40	0.50
2:E:190:MET:HE1	3:F:131:LEU:HA	1.93	0.50
1:A:175:LEU:HD22	1:A:175:LEU:H	1.77	0.50
2:B:439:ASN:N	2:B:439:ASN:ND2	2.59	0.50
1:D:144:LEU:HD21	1:D:182:GLN:HE21	1.75	0.50
3:F:322:PHE:CZ	4:I:3:ARG:HG2	2.47	0.50
2:B:332:GLN:O	2:B:338:TYR:HA	2.12	0.50
1:D:168:ALA:HA	2:E:189:GLN:HE22	1.77	0.50
3:F:240:SER:O	3:F:242:ILE:HG13	2.11	0.49
3:F:119:GLN:HA	3:F:119:GLN:HE21	1.78	0.49
1:A:141:ARG:O	1:A:145:VAL:HG23	2.13	0.49
2:E:266:TRP:HA	2:E:377:THR:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:406:ARG:N	2:E:407:CYS:HA	2.27	0.48
2:B:244:THR:HG22	2:B:245:GLU:HG3	1.94	0.48
3:F:273:LYS:HB2	3:F:311:GLN:HB3	1.95	0.48
2:B:384:GLY:O	2:B:406:ARG:HB2	2.13	0.48
3:F:368:ILE:HG22	3:F:377:TYR:O	2.13	0.48
2:B:385:TRP:HD1	2:B:406:ARG:NH1	2.11	0.48
7:B:503:HOH:O	3:C:138:PRO:HG3	2.13	0.48
2:E:439:ASN:H	2:E:439:ASN:ND2	2.09	0.48
3:C:359:THR:HG21	3:C:363:TYR:O	2.13	0.48
1:A:130:VAL:O	1:A:133:ILE:HG22	2.13	0.47
3:F:298:ALA:C	3:F:300:SER:H	2.17	0.47
2:E:293:TRP:HE1	2:E:296:ASN:ND2	2.12	0.47
2:E:166:ARG:C	2:E:168:LEU:H	2.18	0.47
3:F:307:HIS:CE1	3:F:342:GLY:H	2.32	0.47
3:C:167:TYR:O	3:C:179:LEU:HD12	2.14	0.47
2:E:343:ASN:HA	2:E:354:MET:CE	2.45	0.47
2:B:202:ASN:HD22	2:B:284:ASN:HB2	1.78	0.47
2:B:253:GLN:HE22	2:B:451:SER:HA	1.79	0.47
3:C:361:ASN:N	3:C:361:ASN:HD22	2.11	0.47
3:F:171:PRO:HA	3:F:239:GLN:NE2	2.30	0.47
3:F:250:LEU:HD12	3:F:379:MET:HG3	1.97	0.47
3:F:206:LYS:HD2	3:F:210:GLN:OE1	2.13	0.47
3:F:246:LEU:HD22	3:F:265:PHE:CE1	2.49	0.47
3:C:289:ALA:HB3	3:C:369:TRP:CE2	2.49	0.47
3:C:307:HIS:HE1	3:C:342:GLY:H	1.62	0.47
3:F:321:LYS:O	3:F:338:LYS:HD3	2.14	0.47
3:F:365:ASN:H	3:F:365:ASN:ND2	2.12	0.47
2:B:271:GLN:HA	2:B:271:GLN:HE21	1.80	0.47
3:C:154:GLN:OE1	3:C:387:ILE:HD11	2.15	0.47
3:C:252:ASP:HB2	3:C:377:TYR:OH	2.13	0.47
3:C:307:HIS:CE1	3:C:342:GLY:H	2.33	0.47
2:B:343:ASN:HA	2:B:354:MET:SD	2.55	0.47
2:B:351:ASN:HD22	2:B:351:ASN:C	2.17	0.47
2:E:229:PRO:HB2	2:E:301:GLN:HE22	1.80	0.47
2:B:253:GLN:C	2:B:253:GLN:HE21	2.17	0.46
2:B:267:ASP:HB3	2:B:268:PRO:HD3	1.97	0.46
2:B:178:LYS:HA	2:B:178:LYS:NZ	2.30	0.46
2:B:280:THR:HG22	2:B:280:THR:O	2.16	0.46
3:C:250:LEU:HD11	3:C:344:LEU:HD21	1.98	0.46
2:E:165:LEU:CD1	2:E:168:LEU:HD22	2.41	0.46
3:C:365:ASN:H	3:C:365:ASN:ND2	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:1:NAG:C6	5:L:3:FUC:H5	2.44	0.46
2:B:370:HIS:O	2:B:373:MET:HG2	2.16	0.46
2:B:161:ILE:N	2:B:162:PRO:CD	2.78	0.46
3:F:365:ASN:HD22	3:F:365:ASN:N	2.12	0.46
2:B:351:ASN:ND2	2:B:351:ASN:C	2.70	0.46
2:B:411:ASN:N	2:B:412:PRO:HD3	2.31	0.46
2:B:434:GLY:O	2:B:436:VAL:N	2.48	0.46
3:C:119:GLN:HA	3:C:119:GLN:HE21	1.81	0.46
3:C:321:LYS:O	3:C:338:LYS:HD3	2.15	0.46
3:F:126:GLU:O	3:F:130:GLN:HG3	2.16	0.46
3:C:321:LYS:O	3:C:338:LYS:HB2	2.16	0.45
3:C:297:ASP:HB2	4:G:2:HIS:HD2	1.82	0.45
2:E:190:MET:HE3	3:F:131:LEU:CD1	2.47	0.45
2:B:315:GLU:HA	2:B:320:ASP:O	2.16	0.45
3:F:318:ASP:OD2	3:F:325:ASN:HA	2.16	0.45
3:F:231:GLU:O	3:F:235:LEU:HG	2.16	0.45
2:E:190:MET:CE	3:F:131:LEU:HA	2.46	0.45
3:F:268:GLY:O	3:F:274:TYR:HA	2.16	0.45
1:D:176:LYS:O	1:D:180:ASP:N	2.49	0.45
3:C:298:ALA:HB1	3:C:299:PRO:CD	2.46	0.45
2:E:191:GLU:HG2	2:E:194:ARG:HH11	1.82	0.45
2:B:178:LYS:HA	2:B:178:LYS:HZ3	1.81	0.45
2:E:402:TRP:CH2	2:E:412:PRO:HG2	2.52	0.45
3:F:172:LEU:HD22	3:F:239:GLN:HE21	1.82	0.45
2:B:422:TYR:O	2:B:444:TRP:HB3	2.17	0.44
1:D:176:LYS:HB2	1:D:176:LYS:HZ3	1.82	0.44
2:E:453:LYS:HG3	7:E:475:HOH:O	2.17	0.44
2:B:229:PRO:CB	2:B:301:GLN:HE22	2.30	0.44
3:C:387:ILE:HG12	3:C:388:PRO:HD2	1.98	0.44
1:D:166:SER:HB3	2:E:195:THR:CG2	2.43	0.44
2:E:436:VAL:CG1	2:E:437:TRP:N	2.80	0.44
2:B:172:LEU:HB3	3:C:113:ILE:CD1	2.48	0.44
2:B:402:TRP:CG	2:B:403:TRP:N	2.86	0.44
1:D:181:GLN:OE1	2:E:171:ILE:HB	2.16	0.44
2:E:415:ARG:N	2:E:434:GLY:HA2	2.32	0.44
3:F:389:PHE:C	3:F:391:ARG:N	2.71	0.44
2:B:203:ILE:CD1	3:C:145:ILE:HD11	2.48	0.44
2:B:370:HIS:HE1	2:B:408:HIS:HB2	1.82	0.44
2:B:406:ARG:N	2:B:407:CYS:HA	2.32	0.44
3:F:239:GLN:O	3:F:240:SER:C	2.56	0.44
3:C:361:ASN:N	3:C:361:ASN:ND2	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:195:GLN:HE22	3:C:382:THR:HG21	1.83	0.43
3:F:294:ASP:OD1	3:F:302:LYS:HB2	2.18	0.43
2:E:230:ASP:OD2	2:E:232:SER:HB2	2.18	0.43
2:E:191:GLU:HA	2:E:194:ARG:HD3	1.99	0.43
1:A:136:LEU:HB3	2:B:168:LEU:HD21	2.00	0.43
2:B:378:TYR:HB2	2:B:396:LYS:HG2	2.00	0.43
2:B:381:ASP:HB2	2:B:393:GLN:OE1	2.19	0.43
5:K:2:NAG:O3	5:K:2:NAG:C7	2.66	0.43
1:A:165:CYS:HB3	2:B:193:CYS:HA	2.00	0.43
2:E:230:ASP:HB3	2:E:233:VAL:CG1	2.46	0.43
2:E:402:TRP:CG	2:E:403:TRP:N	2.87	0.43
3:F:364:ASP:HB3	3:F:375:ARG:HG3	1.99	0.43
2:B:175:LEU:O	2:B:179:ILE:HG13	2.19	0.43
2:B:345:TYR:HB2	2:B:354:MET:HE2	2.00	0.43
2:E:423:THR:HG23	2:E:426:MET:CE	2.48	0.43
3:F:307:HIS:HE1	3:F:342:GLY:H	1.65	0.43
2:B:325:HIS:O	2:B:345:TYR:HA	2.19	0.43
3:C:317:ASN:C	3:C:317:ASN:HD22	2.22	0.43
2:B:376:SER:O	2:B:401:GLY:HA2	2.19	0.43
3:C:365:ASN:HD22	3:C:365:ASN:N	2.13	0.43
2:B:431:THR:HG21	4:H:3:ARG:NH2	2.34	0.43
1:D:136:LEU:HG	3:F:111:GLN:NE2	2.34	0.43
3:F:229:GLY:O	3:F:233:ILE:HG13	2.19	0.43
2:B:164:ASN:C	2:B:166:ARG:N	2.72	0.43
3:F:227:TRP:HZ2	3:F:230:ASN:HD21	1.65	0.43
2:B:169:ARG:O	2:B:173:GLU:HG3	2.19	0.42
2:B:177:SER:O	2:B:180:GLN:HB3	2.18	0.42
3:F:217:HIS:O	3:F:224:THR:HG23	2.19	0.42
3:C:251:GLU:HA	3:C:256:ARG:O	2.19	0.42
2:B:190:MET:HG2	3:C:131:LEU:HD13	2.01	0.42
2:B:241:ASP:HB3	2:B:249:TRP:HB2	2.02	0.42
3:C:143:VAL:O	3:C:143:VAL:HG22	2.19	0.42
1:D:142:ALA:C	1:D:144:LEU:H	2.22	0.42
3:F:276:LEU:C	3:F:276:LEU:CD2	2.88	0.42
3:C:114:TYR:CD2	3:C:115:ASN:ND2	2.88	0.42
3:F:143:VAL:O	3:F:143:VAL:HG23	2.19	0.42
2:B:345:TYR:CD2	2:B:351:ASN:HB2	2.54	0.42
3:C:96:TYR:O	3:C:97:GLU:HB3	2.20	0.42
5:L:1:NAG:C6	5:L:3:FUC:H3	2.41	0.42
1:A:175:LEU:HD22	1:A:175:LEU:N	2.34	0.42
2:B:203:ILE:HD13	3:C:145:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:195:GLN:OE1	3:C:382:THR:CG2	2.67	0.42
2:E:439:ASN:ND2	2:E:439:ASN:N	2.65	0.42
3:F:122:VAL:O	3:F:126:GLU:HG3	2.20	0.42
3:F:192:THR:HG21	3:F:236:ILE:HD13	2.02	0.42
1:D:135:LEU:HD13	1:D:135:LEU:C	2.40	0.42
2:E:190:MET:HE3	3:F:131:LEU:HD12	2.01	0.42
3:F:298:ALA:O	3:F:300:SER:N	2.53	0.42
3:C:137:GLU:HA	3:C:138:PRO:HD3	1.87	0.42
3:C:250:LEU:HD12	3:C:379:MET:HG3	2.01	0.42
2:E:327:GLY:HA3	2:E:344:LYS:HE2	2.01	0.42
2:E:241:ASP:OD2	2:E:453:LYS:NZ	2.51	0.41
1:A:175:LEU:O	1:A:179:GLU:HG3	2.20	0.41
2:B:233:VAL:CG1	2:B:234:LYS:N	2.82	0.41
3:C:195:GLN:HB3	3:C:384:MET:HB2	2.01	0.41
3:C:338:LYS:O	3:C:338:LYS:HG2	2.20	0.41
3:C:273:LYS:HB2	3:C:311:GLN:HB3	2.03	0.41
1:A:188:VAL:CG2	2:B:167:VAL:HG21	2.48	0.41
2:E:439:ASN:HD22	2:E:439:ASN:N	2.10	0.41
2:B:296:ASN:HB3	2:B:338:TYR:CE1	2.56	0.41
3:C:277:THR:HA	3:C:308:ASN:OD1	2.21	0.41
2:E:180:GLN:HA	2:E:183:GLU:OE1	2.20	0.41
3:F:291:ASP:O	3:F:302:LYS:HE2	2.21	0.41
1:A:130:VAL:C	1:A:133:ILE:HG22	2.42	0.41
2:B:183:GLU:O	2:B:187:SER:HB2	2.21	0.41
2:B:385:TRP:CD1	2:B:406:ARG:NH1	2.89	0.41
2:E:168:LEU:HD23	3:F:110:LEU:HD13	2.02	0.41
2:E:245:GLU:O	2:E:246:ASN:HB2	2.21	0.41
2:E:411:ASN:N	2:E:412:PRO:HD3	2.36	0.41
2:B:309:GLU:OE1	2:B:325:HIS:HE1	2.04	0.41
2:B:408:HIS:O	4:H:1:GLY:N	2.53	0.41
2:E:415:ARG:H	2:E:434:GLY:H	1.69	0.41
2:B:238:VAL:HG21	2:B:250:THR:HG23	2.04	0.40
2:E:321:LYS:HE2	2:E:321:LYS:HB3	1.89	0.40
2:B:245:GLU:O	2:B:246:ASN:HB2	2.22	0.40
3:C:124:LEU:O	3:C:128:VAL:HG23	2.20	0.40
2:E:170:SER:OG	2:E:171:ILE:N	2.53	0.40
2:E:229:PRO:HG2	2:E:230:ASP:H	1.85	0.40
2:B:317:TRP:CE3	2:B:448:ARG:HD3	2.57	0.40
3:C:215:PHE:HA	7:C:408:HOH:O	2.20	0.40
3:F:387:ILE:CD1	3:F:391:ARG:HG2	2.50	0.40
3:C:184:ILE:HA	3:C:189:ASN:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:206:LYS:HB3	3:C:210:GLN:HB2	2.04	0.40
2:E:244:THR:O	2:E:245:GLU:C	2.59	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	62/66 (94%)	58 (94%)	4 (6%)	0	100	100
1	D	52/66 (79%)	46 (88%)	5 (10%)	1 (2%)	8	10
2	B	296/313 (95%)	265 (90%)	27 (9%)	4 (1%)	11	15
2	E	293/313 (94%)	275 (94%)	14 (5%)	4 (1%)	11	15
3	C	297/311 (96%)	274 (92%)	19 (6%)	4 (1%)	12	17
3	F	283/311 (91%)	264 (93%)	17 (6%)	2 (1%)	22	32
4	G	2/4 (50%)	2 (100%)	0	0	100	100
4	H	2/4 (50%)	2 (100%)	0	0	100	100
4	I	2/4 (50%)	2 (100%)	0	0	100	100
4	J	2/4 (50%)	2 (100%)	0	0	100	100
All	All	1291/1396 (92%)	1190 (92%)	86 (7%)	15 (1%)	13	19

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	281	ASP
2	B	399	GLY
3	C	393	THR
2	E	167	VAL
2	E	281	ASP

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Mol	Chain	Res	Type
3	F	241	ALA
2	B	256	GLN
3	C	370	ALA
3	C	198	LEU
1	D	137	GLN
2	E	256	GLN
3	C	199	ASP
3	F	299	PRO
2	B	435	VAL
2	E	171	ILE

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	59/61 (97%)	58 (98%)	1 (2%)	60	78
1	D	50/61 (82%)	49 (98%)	1 (2%)	55	74
2	B	256/271 (94%)	247 (96%)	9 (4%)	36	55
2	E	253/271 (93%)	244 (96%)	9 (4%)	35	54
3	C	250/257 (97%)	238 (95%)	12 (5%)	25	41
3	F	237/257 (92%)	232 (98%)	5 (2%)	53	72
4	G	3/3 (100%)	3 (100%)	0	100	100
4	H	3/3 (100%)	3 (100%)	0	100	100
4	I	3/3 (100%)	3 (100%)	0	100	100
4	J	3/3 (100%)	3 (100%)	0	100	100
All	All	1117/1190 (94%)	1080 (97%)	37 (3%)	38	57

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	LEU
2	B	178	LYS
2	B	196	PRO

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Mol	Chain	Res	Type
2	B	210	GLU
2	B	253	GLN
2	B	301	GLN
2	B	304	ARG
2	B	351	ASN
2	B	421	GLN
2	B	439	ASN
3	C	104	ASP
3	C	107	ILE
3	C	118	ASN
3	C	143	VAL
3	C	176	GLN
3	C	297	ASP
3	C	317	ASN
3	C	325	ASN
3	C	365	ASN
3	C	374	THR
3	C	382	THR
3	C	383	THR
1	D	176	LYS
2	E	190	MET
2	E	210	GLU
2	E	234	LYS
2	E	253	GLN
2	E	280	THR
2	E	301	GLN
2	E	346	ARG
2	E	351	ASN
2	E	359	GLN
3	F	177	GLN
3	F	317	ASN
3	F	325	ASN
3	F	365	ASN
3	F	383	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	139	ASN
1	A	184	GLN
1	A	187	GLN

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Mol	Chain	Res	Type
2	B	189	GLN
2	B	202	ASN
2	B	253	GLN
2	B	271	GLN
2	B	296	ASN
2	B	301	GLN
2	B	325	HIS
2	B	339	GLN
2	B	351	ASN
2	B	421	GLN
2	B	439	ASN
3	C	111	GLN
3	C	115	ASN
3	C	117	ASN
3	C	118	ASN
3	C	119	GLN
3	C	134	GLN
3	C	136	GLN
3	C	163	GLN
3	C	176	GLN
3	C	177	GLN
3	C	230	ASN
3	C	239	GLN
3	C	254	ASN
3	C	307	HIS
3	C	317	ASN
3	C	319	ASN
3	C	325	ASN
3	C	350	GLN
3	C	361	ASN
3	C	365	ASN
1	D	143	GLN
1	D	182	GLN
1	D	184	GLN
2	E	189	GLN
2	E	202	ASN
2	E	253	GLN
2	E	271	GLN
2	E	296	ASN
2	E	301	GLN
2	E	339	GLN
2	E	351	ASN

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Mol	Chain	Res	Type
2	E	359	GLN
2	E	408	HIS
2	E	421	GLN
2	E	439	ASN
3	F	111	GLN
3	F	115	ASN
3	F	117	ASN
3	F	118	ASN
3	F	119	GLN
3	F	123	ASN
3	F	130	GLN
3	F	144	GLN
3	F	176	GLN
3	F	230	ASN
3	F	239	GLN
3	F	254	ASN
3	F	307	HIS
3	F	317	ASN
3	F	319	ASN
3	F	325	ASN
3	F	350	GLN
3	F	365	ASN
4	G	2	HIS
4	I	2	HIS

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 ⓘ

6 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	$\# Z > 2$
5	NAG	K	1	2,5	14,14,15	0.66	0	17,19,21	0.77	1 (5%)
5	NAG	K	2	5	14,14,15	0.62	0	17,19,21	0.64	0
5	FUC	K	3	5	10,10,11	0.55	0	14,14,16	0.45	0
5	NAG	L	1	2,5	14,14,15	0.65	0	17,19,21	1.25	2 (11%)
5	NAG	L	2	5	14,14,15	0.62	0	17,19,21	0.84	1 (5%)
5	FUC	L	3	5	10,10,11	0.59	0	14,14,16	0.71	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
5	NAG	K	1	2,5	-	4/6/23/26	0/1/1/1
5	NAG	K	2	5	-	6/6/23/26	0/1/1/1
5	FUC	K	3	5	-	-	0/1/1/1
5	NAG	L	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	L	2	5	-	5/6/23/26	0/1/1/1
5	FUC	L	3	5	-	-	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1	NAG	C3-C4-C5	2.63	114.92	110.24
5	L	2	NAG	C2-N2-C7	-2.18	119.80	122.90
5	K	1	NAG	C2-N2-C7	-2.10	119.91	122.90
5	L	1	NAG	C2-N2-C7	-2.09	119.92	122.90

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	1	NAG	C8-C7-N2-C2
5	K	1	NAG	O7-C7-N2-C2
5	K	2	NAG	C3-C2-N2-C7

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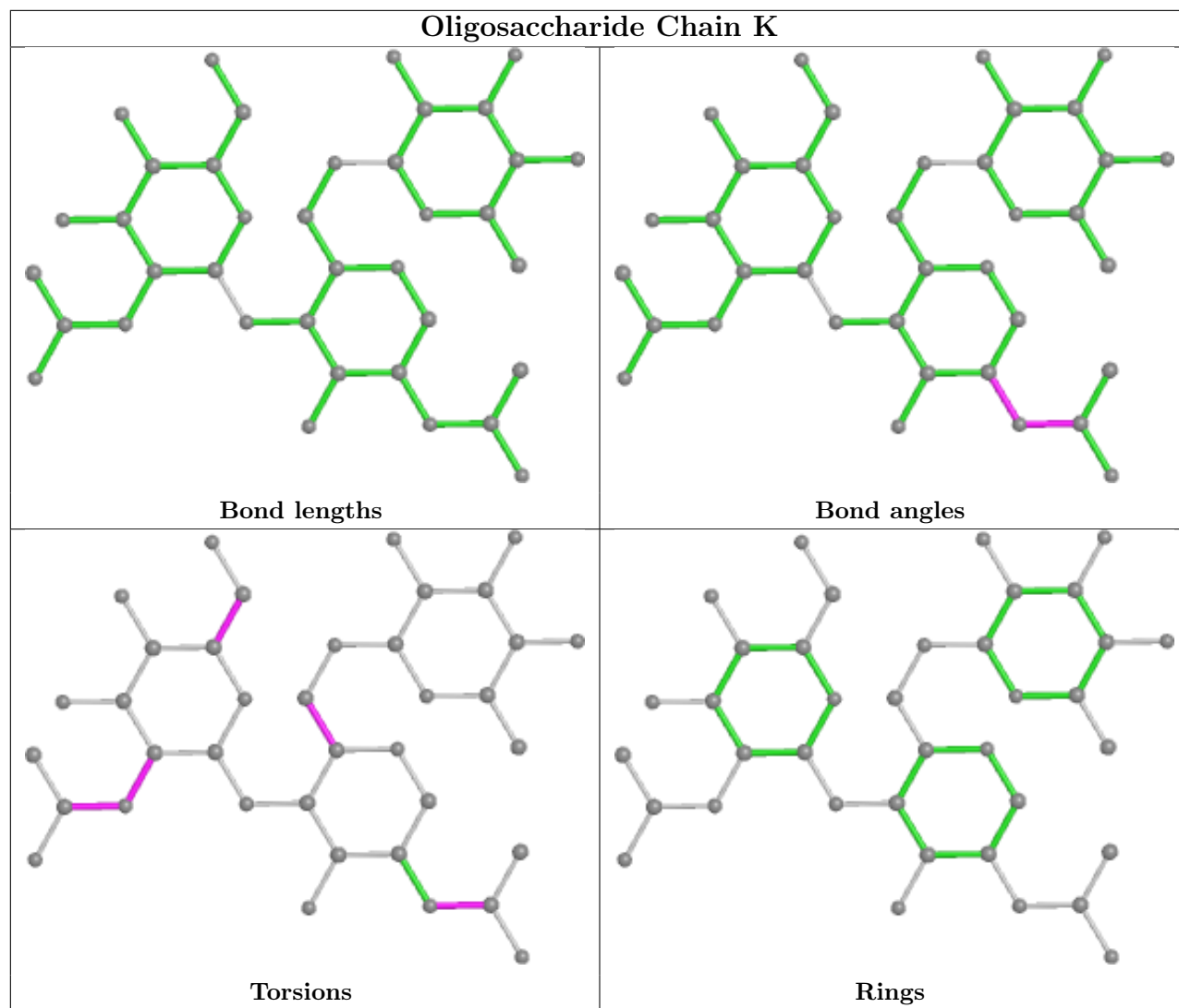
Mol	Chain	Res	Type	Atoms
5	K	2	NAG	C8-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2
5	L	2	NAG	C8-C7-N2-C2
5	L	2	NAG	O7-C7-N2-C2
5	K	2	NAG	O5-C5-C6-O6
5	L	2	NAG	O5-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
5	L	2	NAG	C4-C5-C6-O6
5	L	2	NAG	C3-C2-N2-C7
5	K	2	NAG	C1-C2-N2-C7
5	K	1	NAG	C4-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6

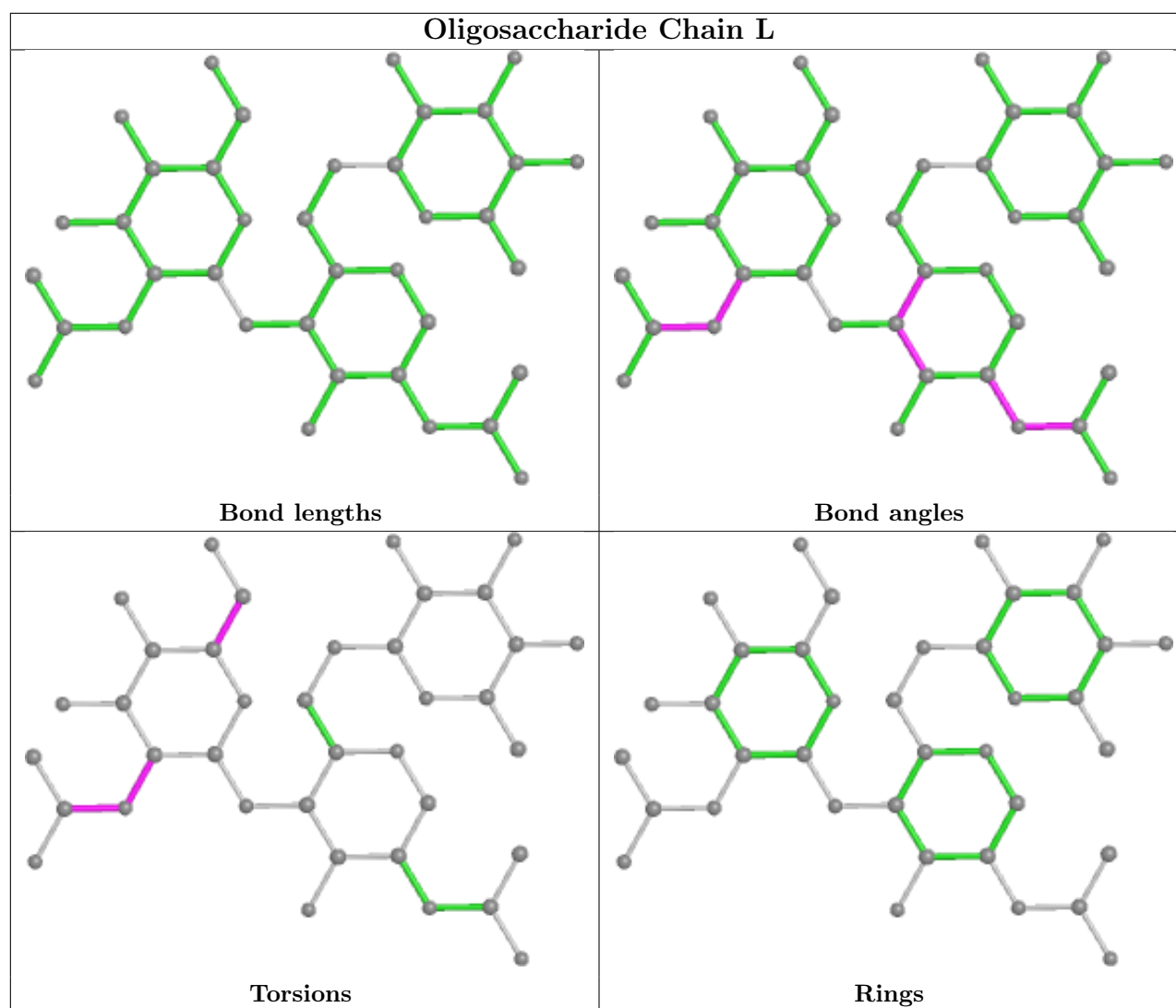
There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	1	NAG	1	0
5	L	1	NAG	9	0
5	L	3	FUC	6	0
5	K	2	NAG	2	0
5	L	2	NAG	3	0

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





5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	64/66 (96%)	0.65	8 (12%) 3 3	25, 65, 100, 107	0
1	D	54/66 (81%)	1.34	21 (38%) 0 0	29, 62, 112, 120	0
2	B	298/313 (95%)	-0.02	5 (1%) 70 68	24, 42, 75, 105	0
2	E	295/313 (94%)	-0.05	13 (4%) 34 33	18, 32, 70, 112	0
3	C	299/311 (96%)	0.26	17 (5%) 23 22	28, 47, 88, 104	0
3	F	285/311 (91%)	0.13	15 (5%) 26 25	23, 39, 79, 114	0
4	G	4/4 (100%)	1.65	1 (25%) 0 0	95, 98, 98, 99	0
4	H	4/4 (100%)	0.85	0 100 100	75, 78, 78, 82	0
4	I	4/4 (100%)	2.83	2 (50%) 0 0	82, 82, 85, 88	0
4	J	4/4 (100%)	-0.03	0 100 100	40, 41, 41, 50	0
All	All	1311/1396 (93%)	0.17	82 (6%) 20 18	18, 41, 91, 120	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	394	ILE	7.2
1	D	140	VAL	6.2
4	I	4	PRO	6.1
3	F	393	THR	5.6
3	F	297	ASP	5.3
1	D	185	LEU	5.1
1	D	180	ASP	4.8
2	E	459	PRO	4.5
1	D	139	ASN	4.5
3	C	360	PRO	4.4
3	F	299	PRO	4.4
1	D	136	LEU	4.4
1	D	138	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
3	F	110	LEU	4.3
3	C	107	ILE	4.2
3	F	113	ILE	4.1
1	D	135	LEU	4.0
1	D	133	ILE	3.9
1	D	182	GLN	3.9
1	D	142	ALA	3.9
3	C	108	ARG	3.8
1	D	184	GLN	3.8
4	G	1	GLY	3.7
2	E	168	LEU	3.6
3	C	96	TYR	3.6
1	D	179	GLU	3.4
2	E	169	ARG	3.4
3	F	394	ILE	3.4
3	C	393	THR	3.3
1	D	176	LYS	3.3
1	A	127	ILE	3.3
1	D	141	ARG	3.2
3	F	363	TYR	3.0
1	D	186	GLU	3.0
2	B	163	THR	2.9
1	A	128	GLU	2.9
3	C	357	ALA	2.8
3	C	253	TRP	2.8
3	F	115	ASN	2.8
1	D	183	LYS	2.8
2	E	170	SER	2.7
3	C	172	LEU	2.7
3	C	254	ASN	2.7
2	E	167	VAL	2.7
1	A	189	ILE	2.7
4	I	2	HIS	2.7
3	F	111	GLN	2.7
2	E	166	ARG	2.7
1	D	137	GLN	2.7
2	B	458	PHE	2.6
1	A	133	ILE	2.6
1	D	175	LEU	2.5
1	A	185	LEU	2.5
2	B	281	ASP	2.5
2	B	168	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
3	F	361	ASN	2.5
2	E	171	ILE	2.4
2	E	458	PHE	2.4
2	E	175	LEU	2.4
3	F	114	TYR	2.4
1	A	131	GLN	2.4
3	C	105	SER	2.4
1	A	132	HIS	2.3
3	F	374	THR	2.3
1	D	134	GLN	2.3
1	D	145	VAL	2.2
1	A	130	VAL	2.2
3	F	112	GLU	2.2
3	F	296	GLY	2.2
3	C	106	SER	2.2
2	E	281	ASP	2.1
2	B	164	ASN	2.1
3	C	111	GLN	2.1
3	C	109	TYR	2.1
2	E	280	THR	2.1
2	E	165	LEU	2.1
3	C	256	ARG	2.1
1	D	144	LEU	2.1
2	E	173	GLU	2.1
3	C	112	GLU	2.0
3	C	359	THR	2.0
3	F	120	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

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

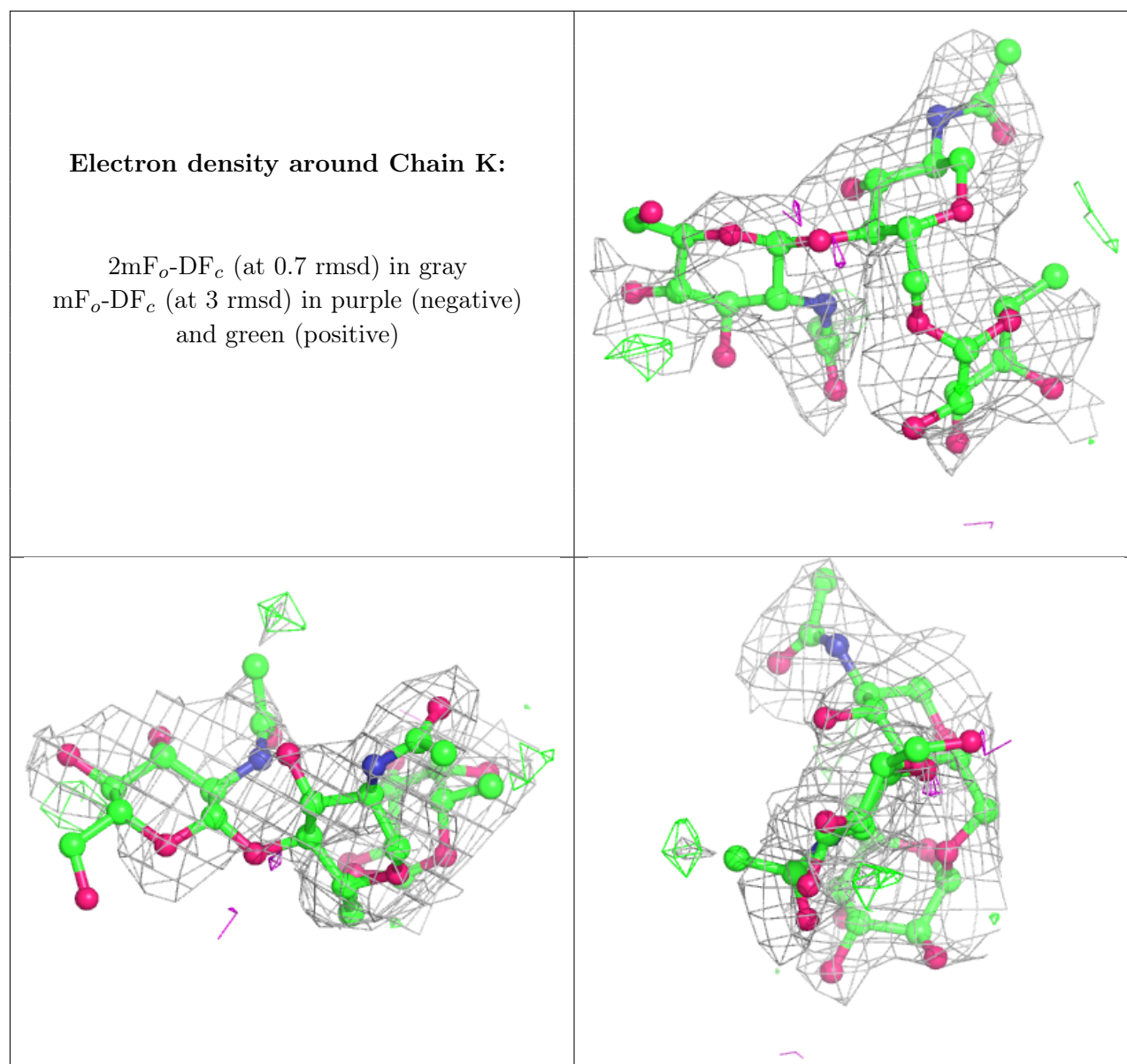
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	L	2	14/15	0.70	0.34	80,83,86,87	0

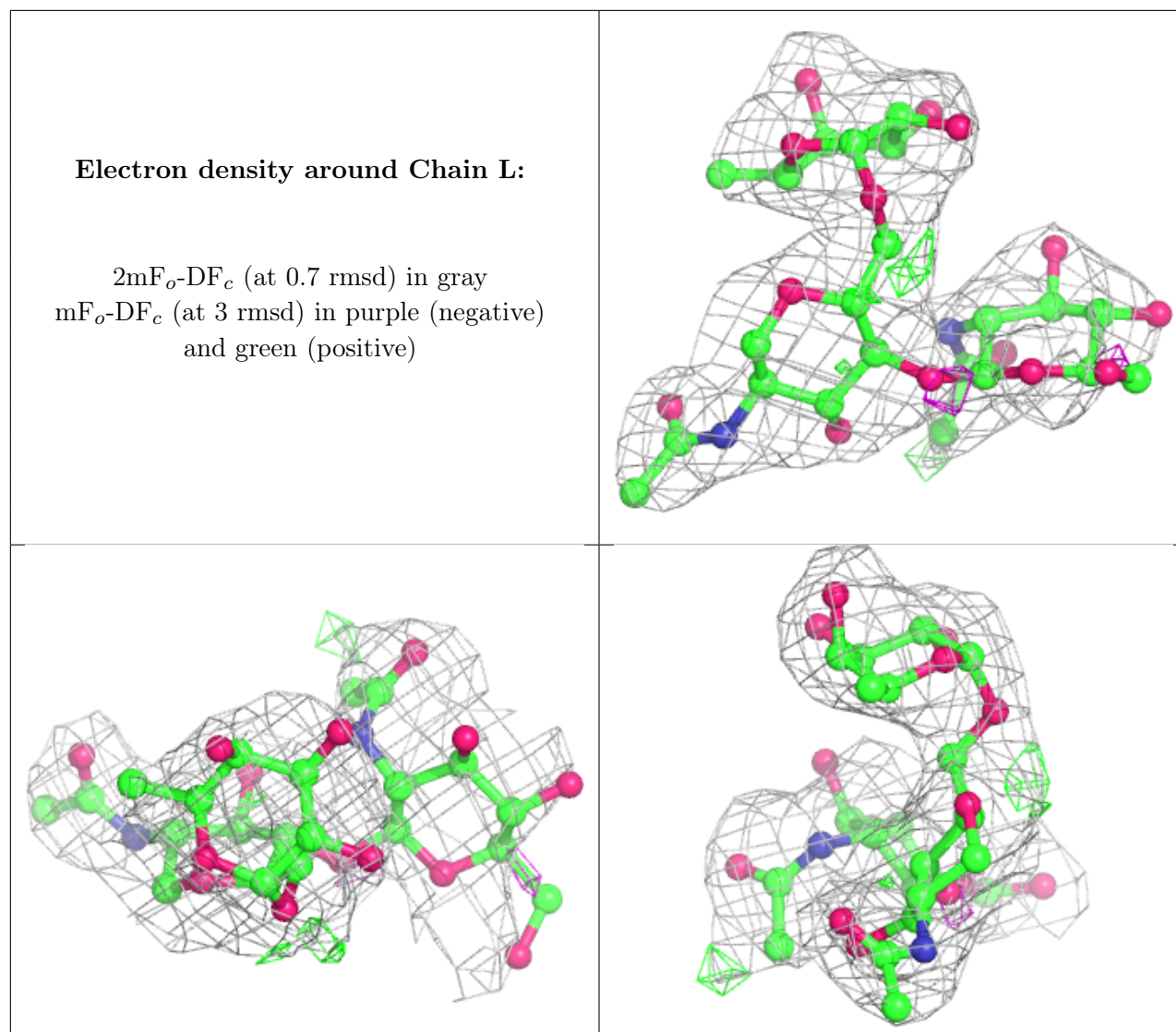
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	K	2	14/15	0.74	0.41	106,108,108,109	0
5	NAG	K	1	14/15	0.76	0.30	89,94,100,103	0
5	FUC	K	3	10/11	0.77	0.34	101,101,102,102	0
5	NAG	L	1	14/15	0.87	0.20	60,64,73,77	0
5	FUC	L	3	10/11	0.91	0.24	72,73,74,74	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.





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
6	CA	E	2	1/1	0.91	0.15	40,40,40,40	0
6	CA	B	2	1/1	0.95	0.16	57,57,57,57	0
6	CA	C	1	1/1	0.96	0.14	49,49,49,49	0
6	CA	F	1	1/1	0.96	0.10	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.