



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:04 AM UTC

PDB ID : 5Z8Y / pdb_00005z8y
Title : Crystal structure of human LRRTM2 in complex with Neurexin 1beta
Authors : Yamagata, A.; Fukai, S.
Deposited on : 2018-02-01
Resolution : 3.40 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 types of validation reports are described at

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

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

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

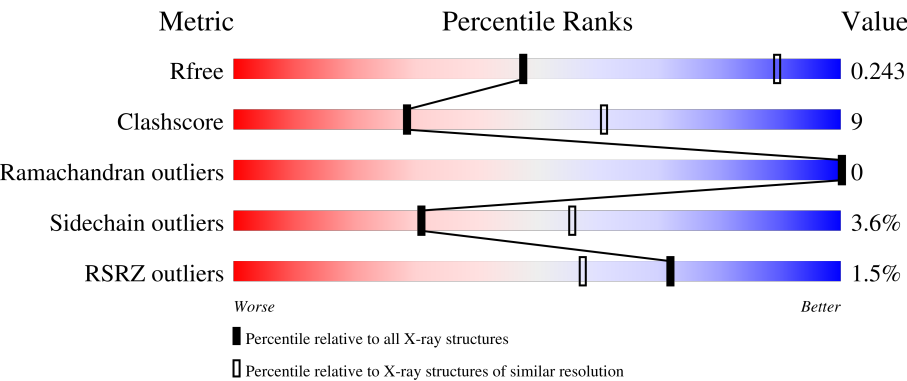
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	346	% 71% 23% • 5%
1	C	346	71% 23% • 5%
1	E	346	% 70% 23% • 5%
1	G	346	% 73% 21% • 5%
2	B	193	3% 69% 20% • 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	193	4% 72% 19% • 8%
2	F	193	% 69% 21% • 8%
2	H	193	3% 70% 20% • 8%
3	I	3	67% 33%
3	J	3	67% 33%
3	K	3	67% 33%
3	L	3	67% 33%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16410 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 Leucine-rich repeat transmembrane neuronal protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2655	1696	465	481	13			
1	C	328	Total	C	N	O	S	0	0	0
			2655	1696	465	481	13			
1	E	328	Total	C	N	O	S	0	0	0
			2655	1696	465	481	13			
1	G	328	Total	C	N	O	S	0	0	0
			2655	1696	465	481	13			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	355	ALA	HIS	engineered mutation	UNP O43300
A	372	GLY	-	expression tag	UNP O43300
A	373	SER	-	expression tag	UNP O43300
A	374	HIS	-	expression tag	UNP O43300
A	375	HIS	-	expression tag	UNP O43300
A	376	HIS	-	expression tag	UNP O43300
A	377	HIS	-	expression tag	UNP O43300
A	378	HIS	-	expression tag	UNP O43300
A	379	HIS	-	expression tag	UNP O43300
C	355	ALA	HIS	engineered mutation	UNP O43300
C	372	GLY	-	expression tag	UNP O43300
C	373	SER	-	expression tag	UNP O43300
C	374	HIS	-	expression tag	UNP O43300
C	375	HIS	-	expression tag	UNP O43300
C	376	HIS	-	expression tag	UNP O43300
C	377	HIS	-	expression tag	UNP O43300
C	378	HIS	-	expression tag	UNP O43300
C	379	HIS	-	expression tag	UNP O43300
E	355	ALA	HIS	engineered mutation	UNP O43300
E	372	GLY	-	expression tag	UNP O43300
E	373	SER	-	expression tag	UNP O43300

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	374	HIS	-	expression tag	UNP O43300
E	375	HIS	-	expression tag	UNP O43300
E	376	HIS	-	expression tag	UNP O43300
E	377	HIS	-	expression tag	UNP O43300
E	378	HIS	-	expression tag	UNP O43300
E	379	HIS	-	expression tag	UNP O43300
G	355	ALA	HIS	engineered mutation	UNP O43300
G	372	GLY	-	expression tag	UNP O43300
G	373	SER	-	expression tag	UNP O43300
G	374	HIS	-	expression tag	UNP O43300
G	375	HIS	-	expression tag	UNP O43300
G	376	HIS	-	expression tag	UNP O43300
G	377	HIS	-	expression tag	UNP O43300
G	378	HIS	-	expression tag	UNP O43300
G	379	HIS	-	expression tag	UNP O43300

- Molecule 2 is a protein called Neurexin-1-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	178	Total	C	N	O	S	0	0	0
			1365	860	244	260	1			
2	D	178	Total	C	N	O	S	0	0	0
			1365	860	244	260	1			
2	F	178	Total	C	N	O	S	0	0	0
			1365	860	244	260	1			
2	H	178	Total	C	N	O	S	0	0	0
			1365	860	244	260	1			

There are 48 discrepancies between the modelled and reference sequences:

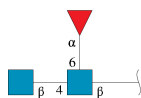
Chain	Residue	Modelled	Actual	Comment	Reference
B	82	ASP	-	expression tag	UNP P58400
B	83	ALA	-	expression tag	UNP P58400
B	84	ALA	-	expression tag	UNP P58400
B	85	SER	-	expression tag	UNP P58400
B	267	GLY	-	expression tag	UNP P58400
B	268	SER	-	expression tag	UNP P58400
B	269	HIS	-	expression tag	UNP P58400
B	270	HIS	-	expression tag	UNP P58400
B	271	HIS	-	expression tag	UNP P58400
B	272	HIS	-	expression tag	UNP P58400
B	273	HIS	-	expression tag	UNP P58400

Continued on next page...

Continued from previous page...

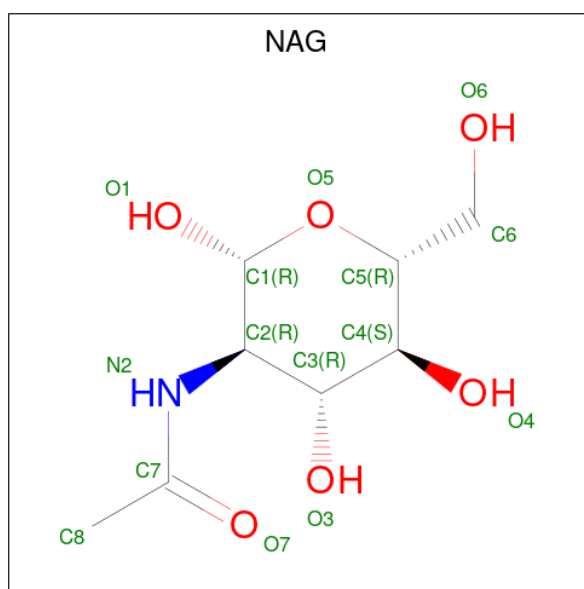
Chain	Residue	Modelled	Actual	Comment	Reference
B	274	HIS	-	expression tag	UNP P58400
D	82	ASP	-	expression tag	UNP P58400
D	83	ALA	-	expression tag	UNP P58400
D	84	ALA	-	expression tag	UNP P58400
D	85	SER	-	expression tag	UNP P58400
D	267	GLY	-	expression tag	UNP P58400
D	268	SER	-	expression tag	UNP P58400
D	269	HIS	-	expression tag	UNP P58400
D	270	HIS	-	expression tag	UNP P58400
D	271	HIS	-	expression tag	UNP P58400
D	272	HIS	-	expression tag	UNP P58400
D	273	HIS	-	expression tag	UNP P58400
D	274	HIS	-	expression tag	UNP P58400
F	82	ASP	-	expression tag	UNP P58400
F	83	ALA	-	expression tag	UNP P58400
F	84	ALA	-	expression tag	UNP P58400
F	85	SER	-	expression tag	UNP P58400
F	267	GLY	-	expression tag	UNP P58400
F	268	SER	-	expression tag	UNP P58400
F	269	HIS	-	expression tag	UNP P58400
F	270	HIS	-	expression tag	UNP P58400
F	271	HIS	-	expression tag	UNP P58400
F	272	HIS	-	expression tag	UNP P58400
F	273	HIS	-	expression tag	UNP P58400
F	274	HIS	-	expression tag	UNP P58400
H	82	ASP	-	expression tag	UNP P58400
H	83	ALA	-	expression tag	UNP P58400
H	84	ALA	-	expression tag	UNP P58400
H	85	SER	-	expression tag	UNP P58400
H	267	GLY	-	expression tag	UNP P58400
H	268	SER	-	expression tag	UNP P58400
H	269	HIS	-	expression tag	UNP P58400
H	270	HIS	-	expression tag	UNP P58400
H	271	HIS	-	expression tag	UNP P58400
H	272	HIS	-	expression tag	UNP P58400
H	273	HIS	-	expression tag	UNP P58400
H	274	HIS	-	expression tag	UNP P58400

- Molecule 3 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
3	I	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	J	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	K	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	L	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



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

Continued on next page...

Continued from previous page...

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

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	C	1	Total	Zn	0	0
			1	1		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		
6	D	1	Total	Ca	0	0
			1	1		
6	F	1	Total	Ca	0	0
			1	1		
6	H	1	Total	Ca	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	O	0	0
			1	1		
7	C	1	Total	O	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	F	1	Total	O	0	0
			1	1		
7	H	1	Total	O	0	0
			1	1		

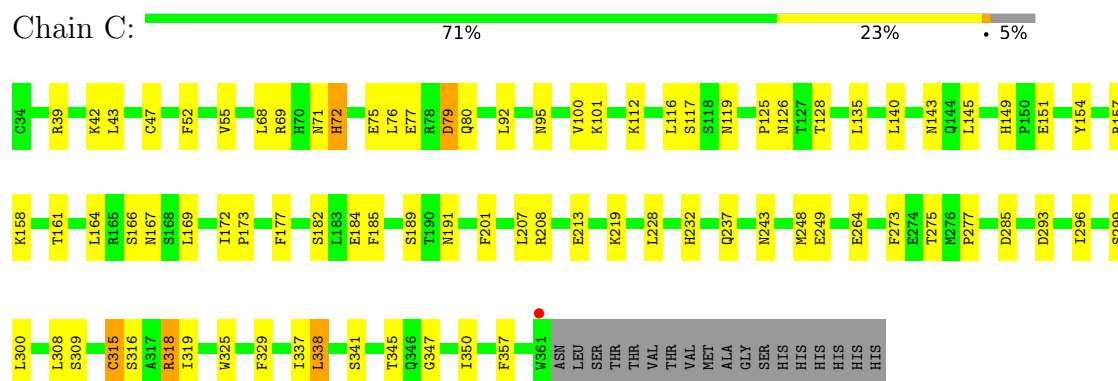
3 Residue-property plots

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.

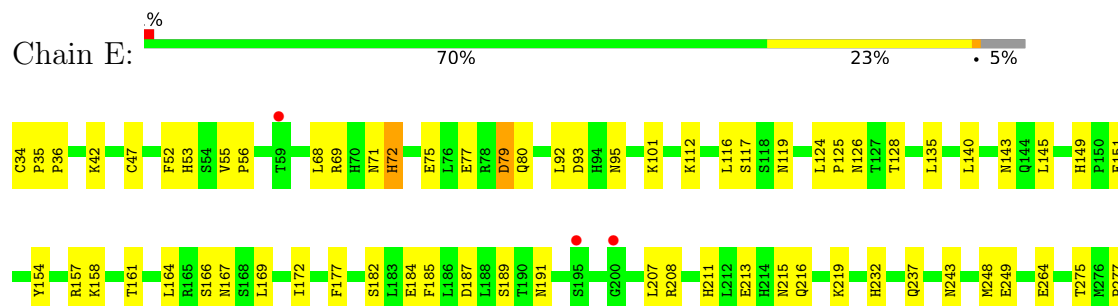
- Molecule 1: Leucine-rich repeat transmembrane neuronal protein 2



- Molecule 1: Leucine-rich repeat transmembrane neuronal protein 2

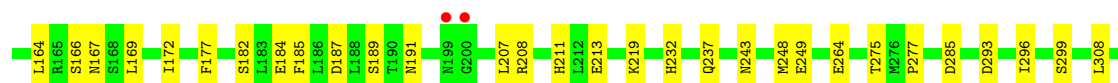
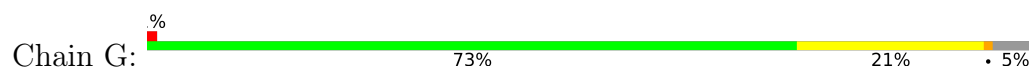


- Molecule 1: Leucine-rich repeat transmembrane neuronal protein 2





- Molecule 1: Leucine-rich repeat transmembrane neuronal protein 2



- Molecule 2: Neurexin-1-beta



- Molecule 2: Neurexin-1-beta



- Molecule 2: Neurexin-1-beta



- Molecule 2: Neurexin-1-beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	99.18Å 99.86Å 109.63Å 91.30° 91.20° 116.47°	Depositor
Resolution (Å)	49.81 – 3.40 49.81 – 3.40	Depositor EDS
% Data completeness (in resolution range)	95.7 (49.81-3.40) 95.7 (49.81-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.209 , 0.241 0.213 , 0.243	Depositor DCC
R_{free} test set	2395 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	75.7	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.095 for -h,-k,l 0.096 for k,h,-l 0.417 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16410	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: NAG, FUC, CA, ZN

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	0.29	0/2716	0.75	0/3679
1	C	0.29	0/2716	0.75	0/3679
1	E	0.28	0/2716	0.75	0/3679
1	G	0.28	0/2716	0.75	0/3679
2	B	0.35	0/1391	0.85	2/1885 (0.1%)
2	D	0.35	0/1391	0.84	2/1885 (0.1%)
2	F	0.34	0/1391	0.83	2/1885 (0.1%)
2	H	0.34	0/1391	0.83	2/1885 (0.1%)
All	All	0.31	0/16428	0.78	8/22256 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	210	ILE	N-CA-C	7.08	118.08	107.75
2	D	210	ILE	N-CA-C	6.89	117.81	107.75
2	F	210	ILE	N-CA-C	6.87	117.78	107.75
2	H	210	ILE	N-CA-C	6.65	117.46	107.75
2	H	88	GLY	N-CA-C	-6.14	103.66	110.96
2	F	88	GLY	N-CA-C	-5.98	103.84	110.96
2	D	88	GLY	N-CA-C	-5.78	104.08	110.96
2	B	88	GLY	N-CA-C	-5.77	104.09	110.96

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	2655	0	2640	57	0
1	C	2655	0	2640	53	0
1	E	2655	0	2640	56	0
1	G	2655	0	2640	49	0
2	B	1365	0	1351	24	0
2	D	1365	0	1351	22	0
2	F	1365	0	1351	23	0
2	H	1365	0	1351	21	0
3	I	38	0	34	0	0
3	J	38	0	34	0	0
3	K	38	0	34	0	0
3	L	38	0	34	0	0
4	A	42	0	39	0	0
4	C	42	0	39	0	0
4	E	42	0	39	0	0
4	G	42	0	39	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	H	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	F	1	0	0	0	0
7	H	1	0	0	0	0
All	All	16410	0	16256	288	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 9.

All (288) 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)
2:H:183:THR:HB	2:H:190:THR:HB	1.61	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:183:THR:HB	2:F:190:THR:HB	1.61	0.81
2:B:183:THR:HB	2:B:190:THR:HB	1.64	0.78
2:D:183:THR:HB	2:D:190:THR:HB	1.65	0.78
1:C:184:GLU:HA	1:C:207:LEU:HA	1.71	0.72
1:C:77:GLU:N	1:C:80:GLN:OE1	2.23	0.72
2:F:105:PRO:HG2	2:F:108:ASP:HB2	1.71	0.71
1:E:184:GLU:HA	1:E:207:LEU:HA	1.71	0.71
2:F:167:GLU:HG2	2:F:193:VAL:HG21	1.73	0.71
2:H:105:PRO:HG2	2:H:108:ASP:HB2	1.72	0.71
1:A:184:GLU:HA	1:A:207:LEU:HA	1.73	0.71
2:H:119:ILE:HD13	2:H:235:LEU:HD12	1.73	0.71
2:D:105:PRO:HG2	2:D:108:ASP:HB2	1.71	0.71
2:F:119:ILE:HD13	2:F:235:LEU:HD12	1.74	0.70
1:G:184:GLU:HA	1:G:207:LEU:HA	1.72	0.70
2:H:167:GLU:HG2	2:H:193:VAL:HG21	1.73	0.70
2:B:105:PRO:HG2	2:B:108:ASP:HB2	1.73	0.69
2:D:167:GLU:HG2	2:D:193:VAL:HG21	1.74	0.69
2:B:167:GLU:HG2	2:B:193:VAL:HG21	1.74	0.69
1:E:315:CYS:N	1:E:341:SER:O	2.23	0.69
1:G:315:CYS:N	1:G:341:SER:O	2.23	0.69
1:C:157:ARG:O	1:C:182:SER:OG	2.10	0.69
1:A:77:GLU:N	1:A:80:GLN:OE1	2.26	0.68
2:B:119:ILE:HD13	2:B:235:LEU:HD12	1.74	0.68
1:G:157:ARG:O	1:G:182:SER:OG	2.12	0.67
2:D:119:ILE:HD13	2:D:235:LEU:HD12	1.75	0.67
1:C:315:CYS:N	1:C:341:SER:O	2.26	0.67
1:A:157:ARG:O	1:A:182:SER:OG	2.11	0.67
1:G:77:GLU:N	1:G:80:GLN:OE1	2.25	0.65
1:E:77:GLU:N	1:E:80:GLN:OE1	2.25	0.65
1:E:157:ARG:O	1:E:182:SER:OG	2.14	0.65
2:F:151:LYS:HD3	2:F:168:SER:HA	1.79	0.65
2:H:151:LYS:HD3	2:H:168:SER:HA	1.79	0.65
2:B:151:LYS:HD3	2:B:168:SER:HA	1.79	0.64
1:A:166:SER:OG	1:C:69:ARG:NH2	2.27	0.63
2:D:151:LYS:HD3	2:D:168:SER:HA	1.79	0.62
2:H:235:LEU:HD22	2:H:242:VAL:HB	1.83	0.61
2:B:107:ASN:OD1	2:B:107:ASN:N	2.32	0.60
2:F:235:LEU:HD22	2:F:242:VAL:HB	1.84	0.60
2:D:235:LEU:HD22	2:D:242:VAL:HB	1.84	0.59
1:A:125:PRO:HG2	1:A:128:THR:HB	1.86	0.58
2:B:235:LEU:HD22	2:B:242:VAL:HB	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:191:LEU:O	2:D:199:ILE:HG12	2.04	0.58
2:F:110:PRO:O	2:F:214:GLN:HG3	2.04	0.58
1:E:264:GLU:OE2	1:G:42:LYS:HE3	2.04	0.57
2:F:191:LEU:O	2:F:199:ILE:HG12	2.05	0.57
2:H:110:PRO:O	2:H:214:GLN:HG3	2.05	0.57
2:H:191:LEU:O	2:H:199:ILE:HG12	2.04	0.56
2:B:191:LEU:O	2:B:199:ILE:HG12	2.05	0.56
1:G:319:ILE:HD12	1:G:350:ILE:HG23	1.88	0.56
1:E:69:ARG:NH2	1:G:166:SER:OG	2.37	0.56
1:G:172:ILE:HD11	1:G:177:PHE:HE2	1.70	0.56
1:A:315:CYS:N	1:A:341:SER:O	2.27	0.56
1:G:172:ILE:HD11	1:G:177:PHE:CE2	2.40	0.56
1:E:125:PRO:HG2	1:E:128:THR:HB	1.87	0.56
1:A:69:ARG:NH2	1:C:166:SER:OG	2.30	0.56
1:E:42:LYS:HE3	1:G:264:GLU:OE2	2.06	0.56
1:G:125:PRO:HG2	1:G:128:THR:HB	1.87	0.56
1:C:126:ASN:HB3	1:C:149:HIS:CG	2.40	0.55
1:E:126:ASN:HB3	1:E:149:HIS:CG	2.42	0.55
1:E:172:ILE:HD11	1:E:177:PHE:CE2	2.41	0.55
1:E:166:SER:OG	1:G:69:ARG:NH2	2.33	0.55
2:D:107:ASN:OD1	2:D:107:ASN:N	2.32	0.55
1:A:126:ASN:HB3	1:A:149:HIS:CG	2.41	0.54
1:E:319:ILE:HD12	1:E:350:ILE:HG23	1.89	0.54
1:A:308:LEU:HB2	1:A:337:ILE:HD13	1.88	0.54
1:G:126:ASN:HB3	1:G:149:HIS:CG	2.42	0.54
1:A:319:ILE:HD12	1:A:350:ILE:HG23	1.89	0.54
1:E:172:ILE:HD11	1:E:177:PHE:HE2	1.72	0.53
2:H:192:GLN:HG3	2:H:198:VAL:HG22	1.90	0.53
1:C:172:ILE:HD11	1:C:177:PHE:CE2	2.44	0.53
1:C:125:PRO:HG2	1:C:128:THR:HB	1.90	0.53
2:D:192:GLN:HG3	2:D:198:VAL:HG22	1.91	0.53
1:E:316:SER:O	1:E:319:ILE:HG12	2.09	0.53
2:B:110:PRO:O	2:B:214:GLN:HG3	2.09	0.53
2:F:192:GLN:HG3	2:F:198:VAL:HG22	1.90	0.53
1:E:143:ASN:HB2	1:E:167:ASN:HD21	1.73	0.52
2:H:179:VAL:H	2:H:194:ASP:HB2	1.74	0.52
1:A:264:GLU:OE2	1:C:42:LYS:HE3	2.09	0.52
1:C:319:ILE:HD12	1:C:350:ILE:HG23	1.90	0.52
1:G:219:LYS:HG3	1:G:243:ASN:HB2	1.90	0.52
2:D:110:PRO:O	2:D:214:GLN:HG3	2.09	0.52
1:E:71:ASN:HB2	1:E:95:ASN:HD21	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:316:SER:O	1:G:319:ILE:HG12	2.09	0.52
1:C:167:ASN:HB2	1:C:191:ASN:HD21	1.75	0.52
1:A:316:SER:O	1:A:319:ILE:HG12	2.09	0.52
1:G:167:ASN:HB2	1:G:191:ASN:HD21	1.74	0.52
2:B:192:GLN:HG3	2:B:198:VAL:HG22	1.92	0.52
1:A:79:ASP:OD1	1:A:79:ASP:N	2.43	0.51
1:A:172:ILE:HD11	1:A:177:PHE:CE2	2.44	0.51
1:C:79:ASP:OD1	1:C:79:ASP:N	2.43	0.51
1:G:143:ASN:HB2	1:G:167:ASN:HD21	1.75	0.51
2:H:107:ASN:OD1	2:H:107:ASN:N	2.33	0.51
1:A:75:GLU:OE2	1:A:101:LYS:NZ	2.43	0.51
1:A:72:HIS:CE1	1:E:53:HIS:HE1	2.28	0.51
1:A:219:LYS:HG3	1:A:243:ASN:HB2	1.93	0.51
2:F:179:VAL:H	2:F:194:ASP:HB2	1.75	0.51
1:C:219:LYS:HG3	1:C:243:ASN:HB2	1.91	0.51
1:C:316:SER:O	1:C:319:ILE:HG12	2.11	0.50
1:E:79:ASP:OD1	1:E:79:ASP:N	2.44	0.50
1:A:53:HIS:CE1	1:E:72:HIS:CE1	2.99	0.50
1:C:126:ASN:HB3	1:C:149:HIS:CD2	2.47	0.49
1:G:140:LEU:HB2	1:G:164:LEU:HD23	1.94	0.49
1:E:167:ASN:HB2	1:E:191:ASN:HD21	1.77	0.49
1:E:219:LYS:HG3	1:E:243:ASN:HB2	1.93	0.49
1:C:308:LEU:HB2	1:C:337:ILE:HD13	1.94	0.49
1:C:75:GLU:OE2	1:C:101:LYS:NZ	2.46	0.49
1:C:189:SER:HB2	1:C:213:GLU:HG2	1.94	0.49
1:G:71:ASN:HB2	1:G:95:ASN:HD21	1.78	0.49
1:A:126:ASN:HB3	1:A:149:HIS:CD2	2.48	0.49
1:A:167:ASN:HB2	1:A:191:ASN:HD21	1.77	0.49
1:G:79:ASP:N	1:G:79:ASP:OD1	2.45	0.49
1:A:42:LYS:HE3	1:C:264:GLU:OE2	2.13	0.48
1:C:112:LYS:HA	1:C:135:LEU:HA	1.95	0.48
1:A:47:CYS:HB2	1:A:68:LEU:HD23	1.95	0.48
1:A:53:HIS:HE1	1:E:72:HIS:CE1	2.31	0.48
1:C:143:ASN:HB2	1:C:167:ASN:HD21	1.78	0.48
1:A:296:ILE:O	1:A:299:SER:OG	2.31	0.48
1:G:308:LEU:HB2	1:G:337:ILE:HD13	1.95	0.48
1:A:112:LYS:HA	1:A:135:LEU:HA	1.96	0.48
1:A:139:ASP:OD1	1:A:141:SER:OG	2.28	0.48
1:A:151:GLU:HG2	1:A:154:TYR:CE2	2.49	0.48
1:A:189:SER:HB2	1:A:213:GLU:HG2	1.96	0.48
2:D:196:TRP:HB3	2:D:197:PRO:HD2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:140:LEU:HB2	1:E:164:LEU:HD23	1.95	0.48
1:C:151:GLU:HG2	1:C:154:TYR:CE2	2.48	0.47
1:E:296:ILE:O	1:E:299:SER:OG	2.30	0.47
1:A:208:ARG:HB3	1:A:232:HIS:CE1	2.49	0.47
1:E:112:LYS:HA	1:E:135:LEU:HA	1.97	0.47
1:E:189:SER:HB2	1:E:213:GLU:HG2	1.96	0.47
1:G:151:GLU:HG2	1:G:154:TYR:CE2	2.49	0.47
1:C:325:TRP:O	1:C:329:PHE:N	2.46	0.47
1:G:112:LYS:HA	1:G:135:LEU:HA	1.97	0.47
1:G:296:ILE:O	1:G:299:SER:OG	2.31	0.47
1:A:92:LEU:HB2	1:A:116:LEU:HD23	1.97	0.47
1:E:316:SER:OG	1:E:318:ARG:HG3	2.15	0.47
1:A:71:ASN:HB2	1:A:95:ASN:HD21	1.80	0.47
1:A:275:THR:O	1:A:277:PRO:HD3	2.15	0.47
2:B:179:VAL:H	2:B:194:ASP:HB2	1.80	0.47
2:B:196:TRP:HB3	2:B:197:PRO:HD2	1.96	0.47
1:G:145:LEU:H	1:G:167:ASN:HD22	1.63	0.47
2:H:196:TRP:HB3	2:H:197:PRO:HD2	1.96	0.47
1:A:325:TRP:O	1:A:329:PHE:N	2.46	0.47
1:A:345:THR:HG22	1:A:357:PHE:CE1	2.50	0.47
1:C:275:THR:O	1:C:277:PRO:HD3	2.16	0.47
1:C:71:ASN:HB2	1:C:95:ASN:HD21	1.79	0.46
2:D:170:ALA:HB3	2:D:196:TRP:CZ3	2.50	0.46
1:G:275:THR:O	1:G:277:PRO:HD3	2.15	0.46
1:C:42:LYS:HB3	1:C:43:LEU:H	1.56	0.46
2:B:116:ARG:NH1	2:B:183:THR:HG23	2.31	0.46
1:C:316:SER:OG	1:C:318:ARG:HG3	2.15	0.46
1:E:308:LEU:HB2	1:E:337:ILE:HD13	1.97	0.46
1:C:296:ILE:O	1:C:299:SER:OG	2.32	0.46
1:E:126:ASN:HB3	1:E:149:HIS:CD2	2.51	0.46
2:D:116:ARG:NH1	2:D:183:THR:HG23	2.31	0.46
1:A:143:ASN:HB2	1:A:167:ASN:HD21	1.81	0.46
1:G:325:TRP:O	1:G:329:PHE:N	2.46	0.46
1:C:117:SER:O	1:C:119:ASN:ND2	2.48	0.46
1:E:275:THR:O	1:E:277:PRO:HD3	2.15	0.46
1:E:325:TRP:O	1:E:329:PHE:N	2.47	0.46
1:E:356:GLY:HA3	2:F:208:LEU:HD21	1.98	0.46
1:A:52:PHE:HB2	1:A:71:ASN:HD22	1.81	0.46
1:C:172:ILE:HD11	1:C:177:PHE:HE2	1.79	0.46
1:C:213:GLU:HB2	1:C:237:GLN:HG2	1.98	0.45
2:D:179:VAL:H	2:D:194:ASP:HB2	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:116:ARG:NH1	2:H:183:THR:HG23	2.31	0.45
1:A:145:LEU:H	1:A:167:ASN:HD22	1.64	0.45
1:A:316:SER:OG	1:A:318:ARG:HG3	2.16	0.45
1:G:126:ASN:HB3	1:G:149:HIS:CD2	2.51	0.45
2:F:196:TRP:HB3	2:F:197:PRO:HD2	1.97	0.45
1:G:52:PHE:HB2	1:G:71:ASN:HD22	1.82	0.45
1:E:151:GLU:HG2	1:E:154:TYR:CE2	2.51	0.45
1:E:345:THR:HG22	1:E:357:PHE:CE1	2.51	0.45
1:E:92:LEU:HB2	1:E:116:LEU:HD23	1.99	0.45
2:F:116:ARG:NH1	2:F:183:THR:HG23	2.31	0.45
1:G:285:ASP:N	1:G:285:ASP:OD1	2.50	0.45
1:E:208:ARG:HB3	1:E:232:HIS:CE1	2.52	0.45
2:B:170:ALA:HB3	2:B:196:TRP:CZ3	2.52	0.44
1:E:285:ASP:N	1:E:285:ASP:OD1	2.50	0.44
2:F:92:ILE:HD13	2:F:231:GLN:HG2	1.99	0.44
2:H:109:ARG:HH11	2:H:136:SER:HB2	1.83	0.44
1:C:47:CYS:HB2	1:C:68:LEU:HD23	1.99	0.44
1:C:52:PHE:HB2	1:C:71:ASN:HD22	1.83	0.44
1:C:208:ARG:HB3	1:C:232:HIS:CE1	2.52	0.44
2:D:94:SER:HB2	2:D:258:ASN:OD1	2.17	0.44
1:E:52:PHE:HB2	1:E:71:ASN:HD22	1.83	0.44
2:F:147:ILE:HG12	2:F:152:ILE:HD12	1.99	0.44
1:G:189:SER:HB2	1:G:213:GLU:HG2	2.00	0.44
1:C:55:VAL:HB	1:C:80:GLN:HE21	1.83	0.44
1:E:47:CYS:HB2	1:E:68:LEU:HD23	1.99	0.44
2:F:94:SER:HB2	2:F:258:ASN:OD1	2.18	0.44
1:G:161:THR:HG22	1:G:185:PHE:HB3	1.99	0.44
2:D:222:LYS:HA	2:D:227:PRO:HG3	2.00	0.44
1:A:126:ASN:OD1	1:A:126:ASN:N	2.51	0.44
1:E:145:LEU:H	1:E:167:ASN:HD22	1.66	0.44
1:G:47:CYS:HB2	1:G:68:LEU:HD23	1.99	0.44
1:G:316:SER:OG	1:G:318:ARG:HG3	2.17	0.44
1:A:72:HIS:CE1	1:E:53:HIS:CE1	3.05	0.43
1:A:172:ILE:HD11	1:A:177:PHE:HE2	1.83	0.43
1:G:213:GLU:HB2	1:G:237:GLN:HG2	1.99	0.43
1:C:345:THR:HG22	1:C:357:PHE:CE1	2.53	0.43
2:F:107:ASN:OD1	2:F:107:ASN:N	2.34	0.43
1:G:92:LEU:HB2	1:G:116:LEU:HD23	2.00	0.43
1:A:213:GLU:HB2	1:A:237:GLN:HG2	2.01	0.43
2:B:94:SER:HB2	2:B:258:ASN:OD1	2.18	0.43
1:A:338:LEU:HD23	1:A:347:GLY:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:HIS:HE1	1:G:53:HIS:HE1	1.66	0.43
2:F:135:SER:OG	2:F:141:ASP:HB2	2.19	0.43
1:C:140:LEU:HB2	1:C:164:LEU:HD23	2.00	0.43
1:G:338:LEU:HD23	1:G:347:GLY:O	2.18	0.43
1:G:169:LEU:H	1:G:191:ASN:HD22	1.67	0.43
2:B:109:ARG:HH11	2:B:136:SER:HB2	1.84	0.43
1:E:338:LEU:HD23	1:E:347:GLY:O	2.18	0.43
1:G:311:ASN:HB2	1:G:313:TRP:NE1	2.34	0.43
2:B:222:LYS:HA	2:B:227:PRO:HG3	2.00	0.43
1:C:273:PHE:CG	1:C:300:LEU:HD21	2.54	0.43
2:F:109:ARG:HH11	2:F:136:SER:HB2	1.84	0.43
2:B:108:ASP:OD1	2:B:108:ASP:N	2.52	0.43
2:B:158:VAL:HG21	2:B:208:LEU:HB2	2.01	0.43
1:C:92:LEU:HB2	1:C:116:LEU:HD23	2.01	0.42
1:E:35:PRO:HA	1:E:36:PRO:HD3	1.90	0.42
1:E:55:VAL:HB	1:E:80:GLN:HE21	1.83	0.42
2:F:250:ASP:HB3	2:F:253:ILE:HG12	2.02	0.42
1:C:201:PHE:HB3	1:C:228:LEU:HD21	2.00	0.42
1:E:126:ASN:OD1	1:E:126:ASN:N	2.51	0.42
1:E:75:GLU:OE2	1:E:101:LYS:NZ	2.52	0.42
1:G:55:VAL:HB	1:G:80:GLN:HE21	1.83	0.42
2:B:123:THR:HB	2:B:228:PHE:HE1	1.84	0.42
1:C:126:ASN:OD1	1:C:126:ASN:N	2.52	0.42
1:A:273:PHE:CG	1:A:300:LEU:HD21	2.55	0.42
1:E:93:ASP:OD1	1:E:93:ASP:N	2.51	0.42
1:E:187:ASP:HA	1:E:211:HIS:HB2	2.02	0.42
2:H:94:SER:HB2	2:H:258:ASN:OD1	2.20	0.42
1:E:161:THR:HG22	1:E:185:PHE:HB3	2.02	0.42
1:E:213:GLU:HB2	1:E:237:GLN:HG2	2.01	0.42
2:F:105:PRO:HA	2:F:106:PRO:HD3	1.90	0.42
1:G:126:ASN:OD1	1:G:126:ASN:N	2.52	0.42
2:H:92:ILE:HD13	2:H:231:GLN:HG2	2.01	0.42
1:G:149:HIS:HA	1:G:150:PRO:HD3	1.94	0.42
1:C:72:HIS:CE1	1:G:53:HIS:HE1	2.38	0.42
2:H:105:PRO:HA	2:H:106:PRO:HD3	1.90	0.42
2:H:135:SER:OG	2:H:141:ASP:HB2	2.20	0.42
2:H:147:ILE:HG12	2:H:152:ILE:HD12	2.01	0.42
1:A:55:VAL:HB	1:A:80:GLN:HE21	1.85	0.42
1:G:117:SER:O	1:G:119:ASN:ND2	2.53	0.42
1:E:215:ASN:HB3	1:E:216:GLN:H	1.74	0.41
1:G:208:ARG:HB3	1:G:232:HIS:CE1	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:158:VAL:HG21	2:D:208:LEU:HB2	2.02	0.41
1:E:55:VAL:HA	1:E:56:PRO:HD3	1.88	0.41
1:A:145:LEU:HD13	1:A:148:LEU:HD21	2.02	0.41
1:A:172:ILE:HA	1:A:173:PRO:HD3	1.90	0.41
1:A:285:ASP:OD1	1:A:285:ASP:N	2.53	0.41
2:B:92:ILE:HD13	2:B:231:GLN:HG2	2.01	0.41
1:C:76:LEU:HD12	1:C:100:VAL:HG22	2.02	0.41
1:E:117:SER:O	1:E:119:ASN:ND2	2.54	0.41
1:A:116:LEU:HB2	1:A:140:LEU:HD23	2.02	0.41
1:C:145:LEU:H	1:C:167:ASN:HD22	1.68	0.41
1:A:161:THR:HG22	1:A:185:PHE:HB3	2.03	0.41
1:A:278:ASN:O	1:A:280:LYS:HG3	2.21	0.41
1:C:285:ASP:OD2	1:C:309:SER:OG	2.38	0.41
1:G:39:ARG:O	1:G:39:ARG:HG3	2.21	0.41
1:C:161:THR:HG22	1:C:185:PHE:HB3	2.03	0.41
1:C:172:ILE:HA	1:C:173:PRO:HD3	1.92	0.41
1:E:169:LEU:H	1:E:191:ASN:HD22	1.69	0.41
1:A:140:LEU:HB2	1:A:164:LEU:HD23	2.02	0.41
2:B:105:PRO:HA	2:B:106:PRO:HD3	1.90	0.41
2:D:108:ASP:OD1	2:D:108:ASP:N	2.53	0.41
1:A:55:VAL:H	1:A:80:GLN:HE21	1.69	0.41
1:A:348:GLU:HG2	2:B:210:ILE:HB	2.03	0.41
2:B:152:ILE:HB	2:B:172:ILE:HG12	2.03	0.41
1:C:169:LEU:H	1:C:191:ASN:HD22	1.69	0.41
1:C:338:LEU:HD23	1:C:347:GLY:O	2.21	0.41
1:E:124:LEU:HA	1:E:125:PRO:HD2	1.94	0.41
1:A:69:ARG:NE	1:A:93:ASP:OD2	2.52	0.41
2:D:135:SER:OG	2:D:141:ASP:HB2	2.22	0.41
2:D:199:ILE:HD13	2:D:199:ILE:N	2.36	0.41
2:D:105:PRO:HA	2:D:106:PRO:HD3	1.90	0.40
1:A:117:SER:O	1:A:119:ASN:ND2	2.54	0.40
1:C:72:HIS:CE1	1:G:53:HIS:CE1	3.09	0.40
1:E:34:CYS:HA	1:E:35:PRO:HD2	1.90	0.40
2:F:182:PHE:HA	2:F:190:THR:O	2.21	0.40
1:A:169:LEU:H	1:A:191:ASN:HD22	1.69	0.40
1:C:39:ARG:O	1:C:39:ARG:HG3	2.20	0.40
2:D:123:THR:HB	2:D:228:PHE:HE1	1.86	0.40
2:F:183:THR:O	2:F:189:ALA:HA	2.22	0.40
2:H:123:THR:HB	2:H:228:PHE:HE1	1.86	0.40
1:G:187:ASP:HA	1:G:211:HIS:HB2	2.03	0.40
2:H:250:ASP:HB3	2:H:253:ILE:HG12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	326/346 (94%)	310 (95%)	16 (5%)	0	100	100
1	C	326/346 (94%)	310 (95%)	16 (5%)	0	100	100
1	E	326/346 (94%)	310 (95%)	16 (5%)	0	100	100
1	G	326/346 (94%)	310 (95%)	16 (5%)	0	100	100
2	B	176/193 (91%)	170 (97%)	6 (3%)	0	100	100
2	D	176/193 (91%)	170 (97%)	6 (3%)	0	100	100
2	F	176/193 (91%)	170 (97%)	6 (3%)	0	100	100
2	H	176/193 (91%)	170 (97%)	6 (3%)	0	100	100
All	All	2008/2156 (93%)	1920 (96%)	88 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	300/316 (95%)	291 (97%)	9 (3%)	36	59
1	C	300/316 (95%)	291 (97%)	9 (3%)	36	59
1	E	300/316 (95%)	291 (97%)	9 (3%)	36	59
1	G	300/316 (95%)	291 (97%)	9 (3%)	36	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	144/155 (93%)	137 (95%)	7 (5%)	22	49
2	D	144/155 (93%)	137 (95%)	7 (5%)	22	49
2	F	144/155 (93%)	137 (95%)	7 (5%)	22	49
2	H	144/155 (93%)	137 (95%)	7 (5%)	22	49
All	All	1776/1884 (94%)	1712 (96%)	64 (4%)	31	56

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	79	ASP
1	A	158	LYS
1	A	248	MET
1	A	249	GLU
1	A	293	ASP
1	A	315	CYS
1	A	318	ARG
1	A	338	LEU
2	B	107	ASN
2	B	171	ILE
2	B	193	VAL
2	B	199	ILE
2	B	212	ASN
2	B	214	GLN
2	B	259	VAL
1	C	72	HIS
1	C	79	ASP
1	C	158	LYS
1	C	248	MET
1	C	249	GLU
1	C	293	ASP
1	C	315	CYS
1	C	318	ARG
1	C	338	LEU
2	D	107	ASN
2	D	171	ILE
2	D	193	VAL
2	D	199	ILE
2	D	212	ASN
2	D	214	GLN
2	D	259	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	72	HIS
1	E	79	ASP
1	E	158	LYS
1	E	248	MET
1	E	249	GLU
1	E	293	ASP
1	E	315	CYS
1	E	318	ARG
1	E	338	LEU
2	F	107	ASN
2	F	171	ILE
2	F	193	VAL
2	F	199	ILE
2	F	212	ASN
2	F	214	GLN
2	F	259	VAL
1	G	72	HIS
1	G	79	ASP
1	G	158	LYS
1	G	248	MET
1	G	249	GLU
1	G	293	ASP
1	G	315	CYS
1	G	318	ARG
1	G	338	LEU
2	H	107	ASN
2	H	171	ILE
2	H	193	VAL
2	H	199	ILE
2	H	212	ASN
2	H	214	GLN
2	H	259	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	134	ASN
1	A	163	HIS
1	A	167	ASN
1	A	191	ASN
1	A	216	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	232	HIS
1	A	290	ASN
1	A	330	GLN
1	A	335	HIS
1	A	340	HIS
1	A	346	GLN
2	B	231	GLN
1	C	95	ASN
1	C	134	ASN
1	C	163	HIS
1	C	167	ASN
1	C	191	ASN
1	C	216	GLN
1	C	232	HIS
1	C	290	ASN
1	C	330	GLN
1	C	335	HIS
1	C	340	HIS
1	C	346	GLN
2	D	231	GLN
1	E	95	ASN
1	E	134	ASN
1	E	163	HIS
1	E	167	ASN
1	E	191	ASN
1	E	214	HIS
1	E	216	GLN
1	E	232	HIS
1	E	290	ASN
1	E	330	GLN
1	E	335	HIS
1	E	340	HIS
1	E	346	GLN
1	G	86	GLN
1	G	95	ASN
1	G	134	ASN
1	G	163	HIS
1	G	167	ASN
1	G	191	ASN
1	G	216	GLN
1	G	232	HIS
1	G	330	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	335	HIS
1	G	346	GLN
2	H	231	GLN

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 ⓘ

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	$\# Z > 2$
3	NAG	I	1	3,2	14,14,15	0.53	0	17,19,21	0.62	0
3	NAG	I	2	3	14,14,15	0.17	0	17,19,21	0.42	0
3	FUC	I	3	3	10,10,11	0.90	0	14,14,16	1.57	2 (14%)
3	NAG	J	1	3,2	14,14,15	0.60	0	17,19,21	0.59	0
3	NAG	J	2	3	14,14,15	0.17	0	17,19,21	0.44	0
3	FUC	J	3	3	10,10,11	0.76	0	14,14,16	1.53	2 (14%)
3	NAG	K	1	3,2	14,14,15	0.47	0	17,19,21	0.56	0
3	NAG	K	2	3	14,14,15	0.14	0	17,19,21	0.46	0
3	FUC	K	3	3	10,10,11	0.80	0	14,14,16	1.31	2 (14%)
3	NAG	L	1	3,2	14,14,15	0.51	0	17,19,21	0.58	0
3	NAG	L	2	3	14,14,15	0.17	0	17,19,21	0.42	0
3	FUC	L	3	3	10,10,11	0.73	0	14,14,16	1.32	2 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	I	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	FUC	I	3	3	-	-	0/1/1/1
3	NAG	J	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	FUC	J	3	3	-	-	0/1/1/1
3	NAG	K	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	FUC	K	3	3	-	-	0/1/1/1
3	NAG	L	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	FUC	L	3	3	-	-	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	3	FUC	C1-O5-C5	3.74	121.80	112.97
3	J	3	FUC	C1-O5-C5	3.65	121.59	112.97
3	I	3	FUC	O5-C5-C4	3.37	115.63	109.55
3	K	3	FUC	C1-O5-C5	3.20	120.52	112.97
3	L	3	FUC	C1-O5-C5	3.00	120.05	112.97
3	J	3	FUC	O5-C5-C4	3.00	114.94	109.55
3	L	3	FUC	O5-C5-C4	2.73	114.46	109.55
3	K	3	FUC	O5-C5-C4	2.33	113.75	109.55

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	2	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6

Continued on next page...

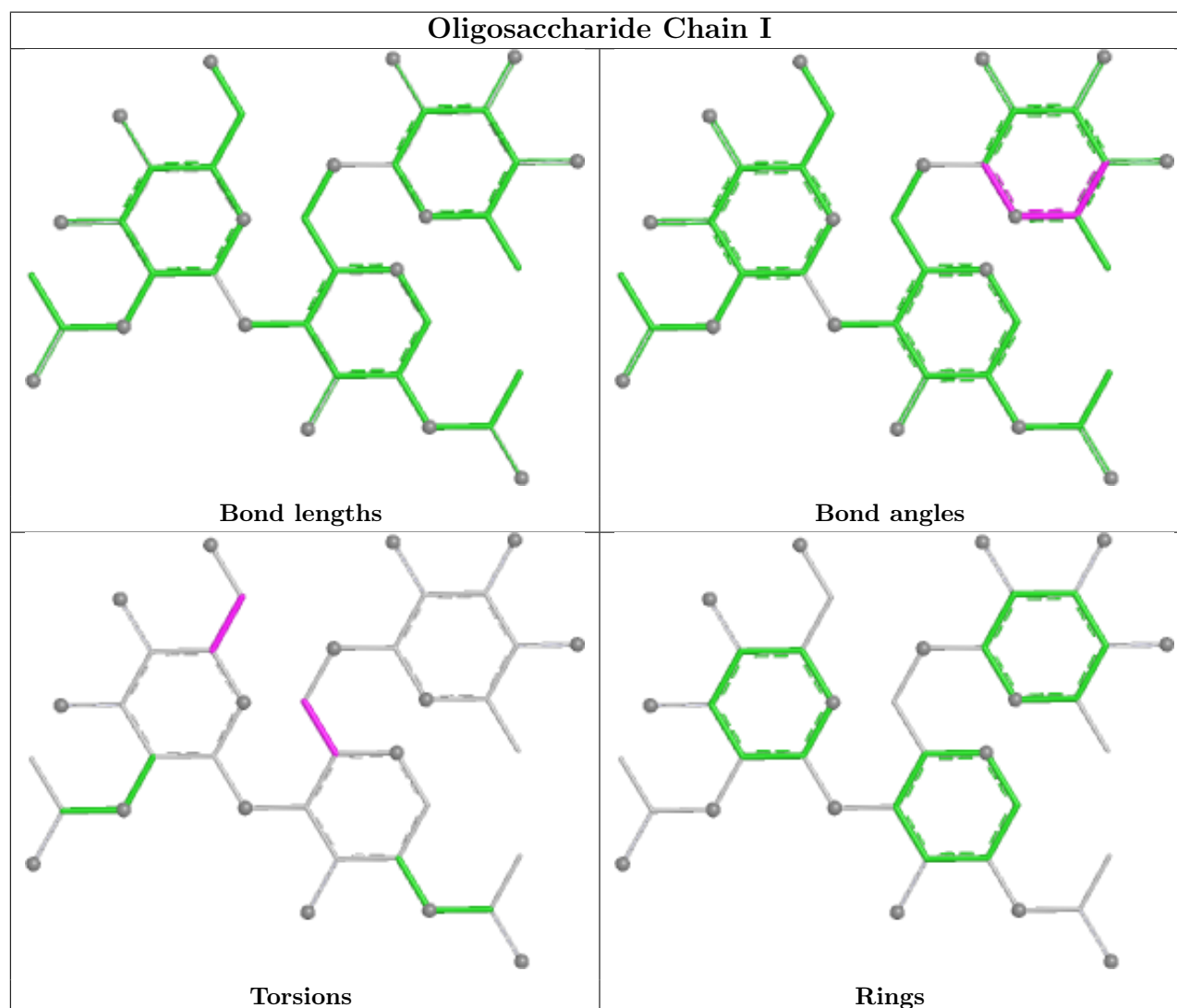
Continued from previous page...

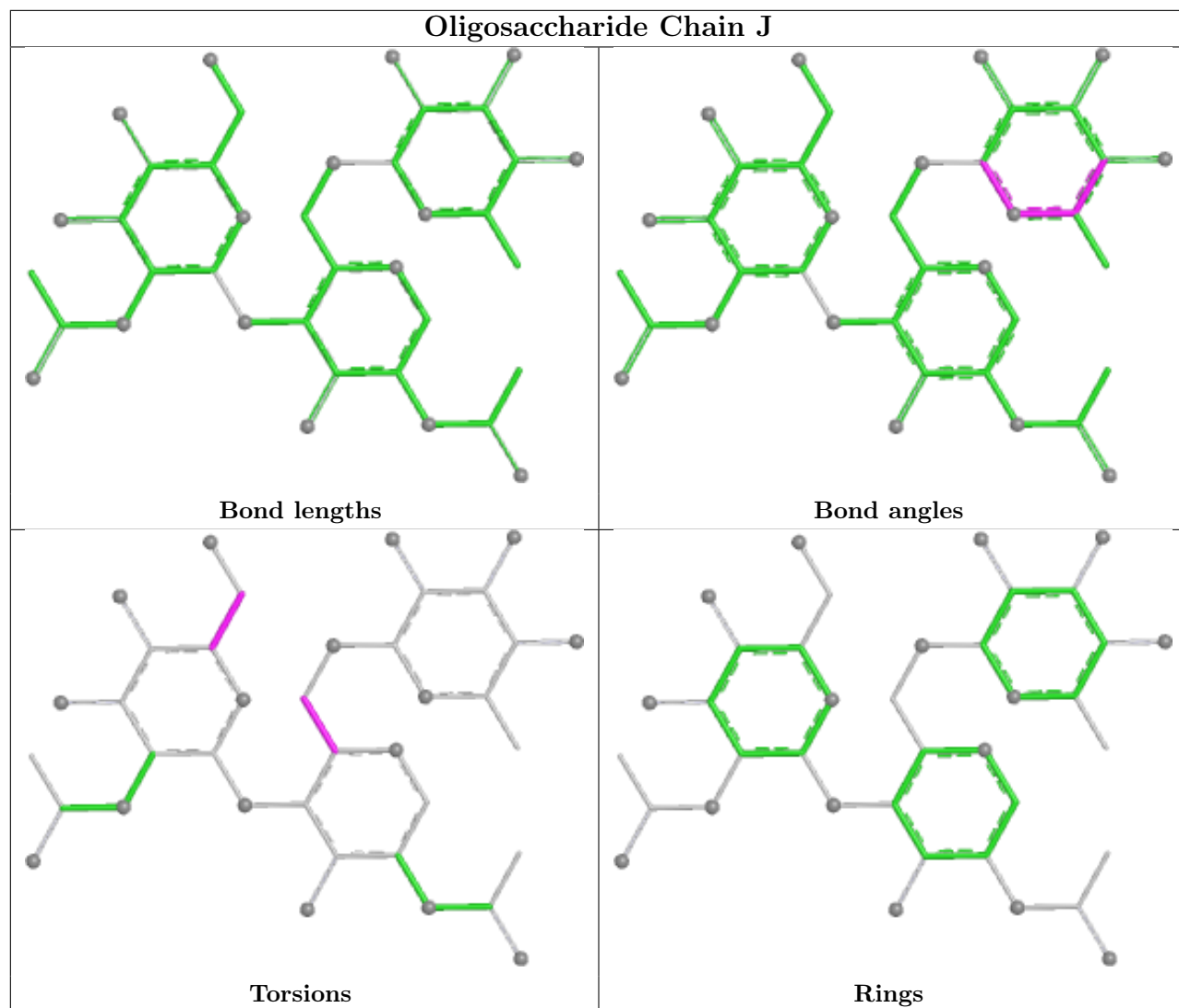
Mol	Chain	Res	Type	Atoms
3	I	2	NAG	C4-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6

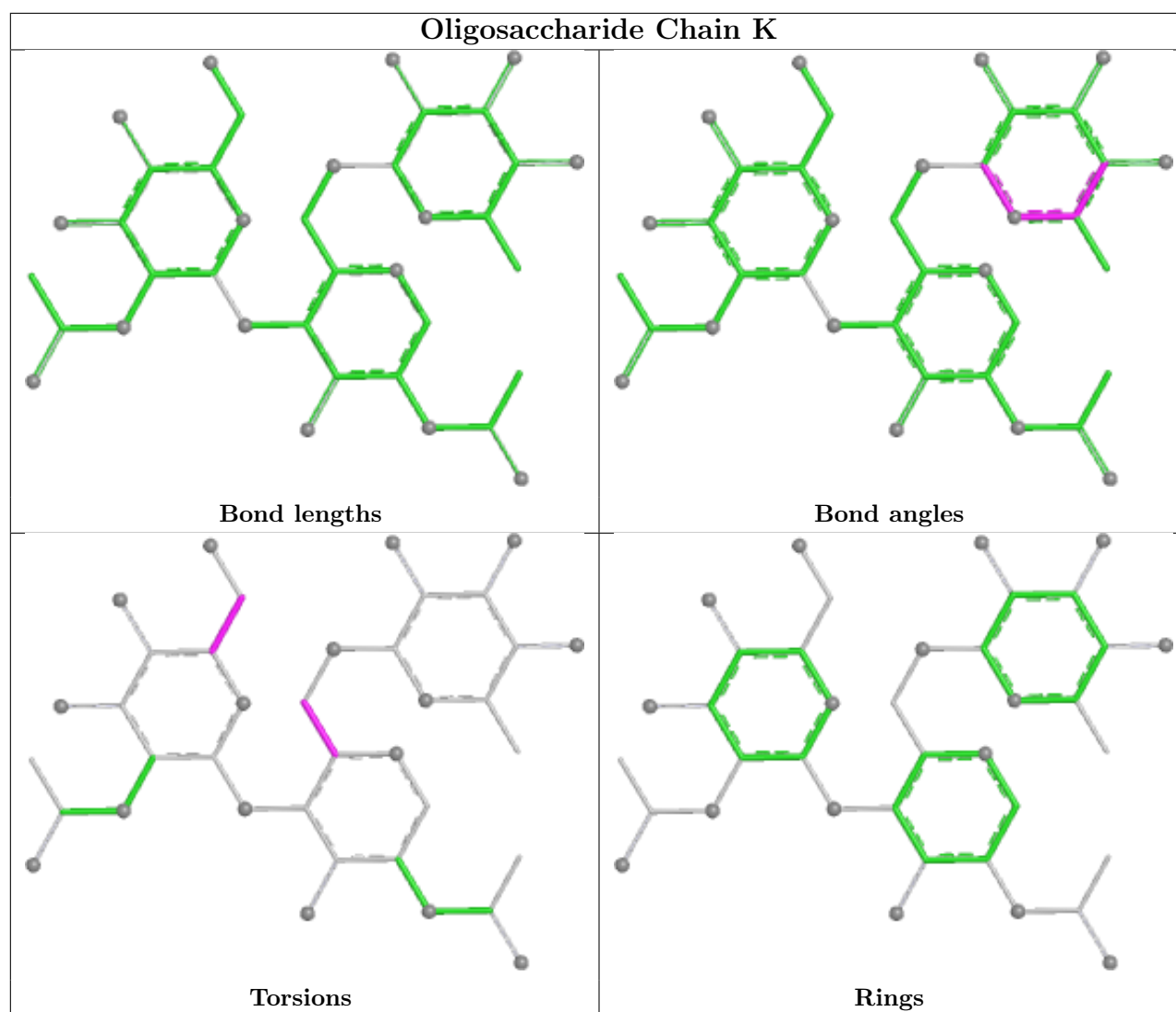
There are no ring outliers.

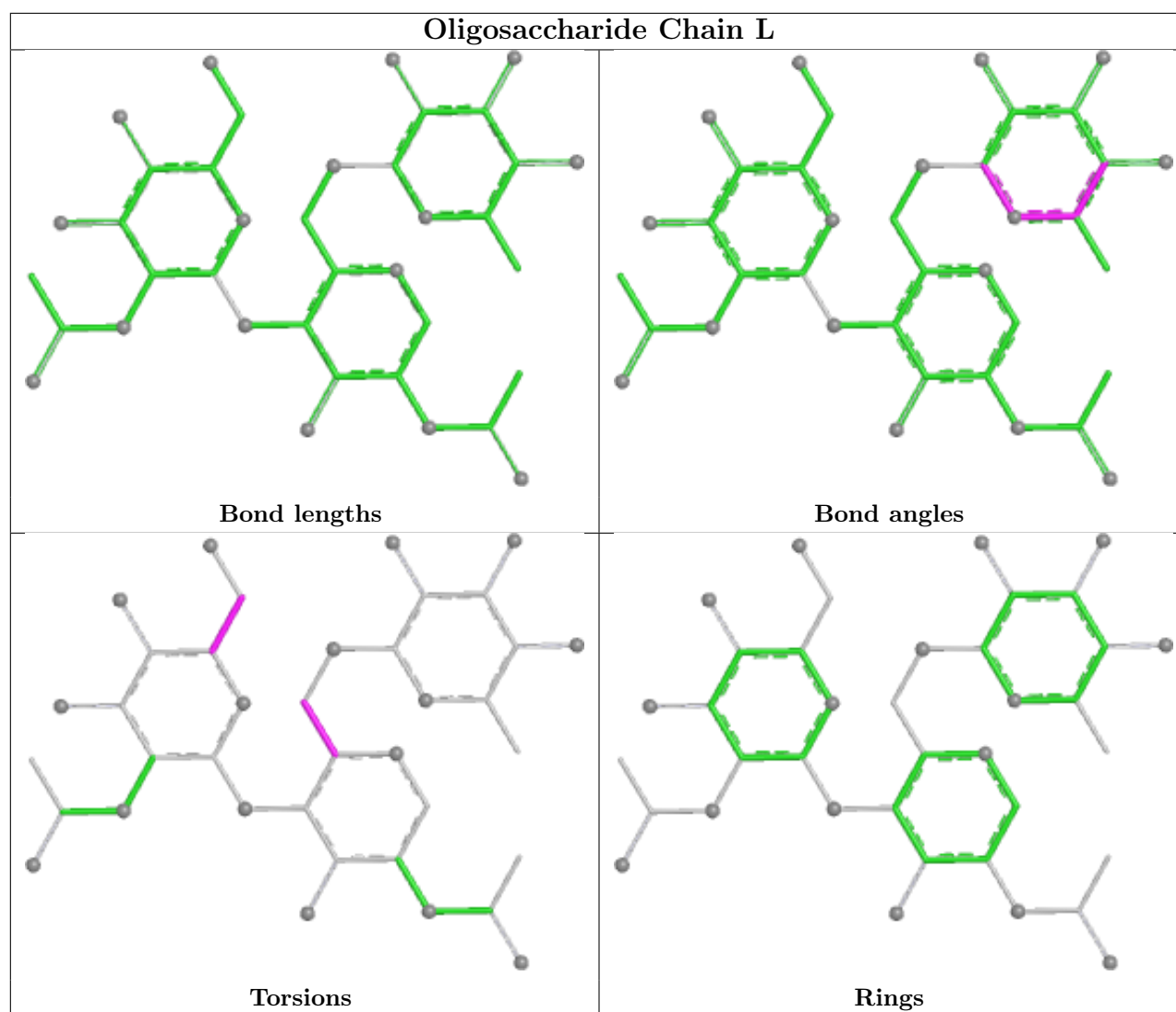
No monomer is involved in short contacts.

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 [i](#)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	E	1000	1	14,14,15	0.30	0	17,19,21	0.34	0
4	NAG	G	1001	1	14,14,15	0.70	1 (7%)	17,19,21	1.00	1 (5%)
4	NAG	G	1000	1	14,14,15	0.30	0	17,19,21	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	401	1	14,14,15	0.27	0	17,19,21	0.34	0
4	NAG	C	403	1	14,14,15	0.33	0	17,19,21	0.48	0
4	NAG	E	1001	1	14,14,15	0.68	1 (7%)	17,19,21	1.01	1 (5%)
4	NAG	E	1002	1	14,14,15	0.31	0	17,19,21	0.51	0
4	NAG	G	1002	1	14,14,15	0.31	0	17,19,21	0.51	0
4	NAG	C	402	1	14,14,15	0.61	1 (7%)	17,19,21	1.01	1 (5%)
4	NAG	A	401	1	14,14,15	0.29	0	17,19,21	0.34	0
4	NAG	A	403	1	14,14,15	0.30	0	17,19,21	0.50	0
4	NAG	A	402	1	14,14,15	0.60	0	17,19,21	1.04	1 (5%)

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	E	1000	1	-	2/6/23/26	0/1/1/1
4	NAG	G	1001	1	-	2/6/23/26	0/1/1/1
4	NAG	G	1000	1	-	2/6/23/26	0/1/1/1
4	NAG	C	401	1	-	2/6/23/26	0/1/1/1
4	NAG	C	403	1	-	0/6/23/26	0/1/1/1
4	NAG	E	1001	1	-	2/6/23/26	0/1/1/1
4	NAG	E	1002	1	-	1/6/23/26	0/1/1/1
4	NAG	G	1002	1	-	1/6/23/26	0/1/1/1
4	NAG	C	402	1	-	2/6/23/26	0/1/1/1
4	NAG	A	401	1	-	2/6/23/26	0/1/1/1
4	NAG	A	403	1	-	0/6/23/26	0/1/1/1
4	NAG	A	402	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1001	NAG	C1-C2	2.26	1.55	1.52
4	E	1001	NAG	C1-C2	2.18	1.55	1.52
4	C	402	NAG	C1-C2	2.07	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	402	NAG	C1-O5-C5	3.81	117.29	112.19
4	C	402	NAG	C1-O5-C5	3.68	117.12	112.19
4	E	1001	NAG	C1-O5-C5	3.62	117.03	112.19
4	G	1001	NAG	C1-O5-C5	3.56	116.95	112.19

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	401	NAG	O5-C5-C6-O6
4	A	402	NAG	O5-C5-C6-O6
4	C	402	NAG	O5-C5-C6-O6
4	E	1000	NAG	O5-C5-C6-O6
4	E	1001	NAG	O5-C5-C6-O6
4	G	1001	NAG	O5-C5-C6-O6
4	C	401	NAG	O5-C5-C6-O6
4	G	1000	NAG	O5-C5-C6-O6
4	A	401	NAG	C4-C5-C6-O6
4	A	402	NAG	C4-C5-C6-O6
4	G	1001	NAG	C4-C5-C6-O6
4	E	1000	NAG	C4-C5-C6-O6
4	E	1001	NAG	C4-C5-C6-O6
4	C	401	NAG	C4-C5-C6-O6
4	C	402	NAG	C4-C5-C6-O6
4	G	1000	NAG	C4-C5-C6-O6
4	E	1002	NAG	C1-C2-N2-C7
4	G	1002	NAG	C1-C2-N2-C7

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	328/346 (94%)	0.02	4 (1%) 76 63	46, 74, 125, 192	0
1	C	328/346 (94%)	0.02	1 (0%) 90 84	47, 74, 126, 179	0
1	E	328/346 (94%)	-0.02	4 (1%) 76 63	48, 77, 121, 173	0
1	G	328/346 (94%)	-0.03	4 (1%) 76 63	48, 77, 120, 171	0
2	B	178/193 (92%)	0.19	5 (2%) 55 41	59, 89, 136, 164	0
2	D	178/193 (92%)	0.30	7 (3%) 43 31	62, 90, 133, 148	0
2	F	178/193 (92%)	0.29	1 (0%) 85 75	65, 117, 161, 171	0
2	H	178/193 (92%)	0.37	5 (2%) 55 41	66, 114, 155, 168	0
All	All	2024/2156 (93%)	0.10	31 (1%) 72 57	46, 84, 140, 192	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	164	ALA	3.6
2	H	186	GLY	3.3
2	D	222	LYS	3.0
2	B	199	ILE	2.9
1	E	361	TRP	2.9
1	G	361	TRP	2.9
2	D	199	ILE	2.8
2	B	195	SER	2.8
1	G	59	THR	2.8
2	B	189	ALA	2.7
1	A	59	THR	2.7
1	A	361	TRP	2.7
1	E	59	THR	2.6
2	D	195	SER	2.6
1	E	200	GLY	2.5
2	D	169	ASN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	361	TRP	2.5
2	D	189	ALA	2.4
1	G	200	GLY	2.3
2	F	218	ILE	2.3
1	G	199	ASN	2.3
1	A	58	ALA	2.3
2	D	221	GLY	2.2
1	A	56	PRO	2.1
2	B	106	PRO	2.1
2	D	98	GLY	2.1
2	H	209	THR	2.1
2	H	154	VAL	2.0
1	E	195	SER	2.0
2	B	172	ILE	2.0
2	H	218	ILE	2.0

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

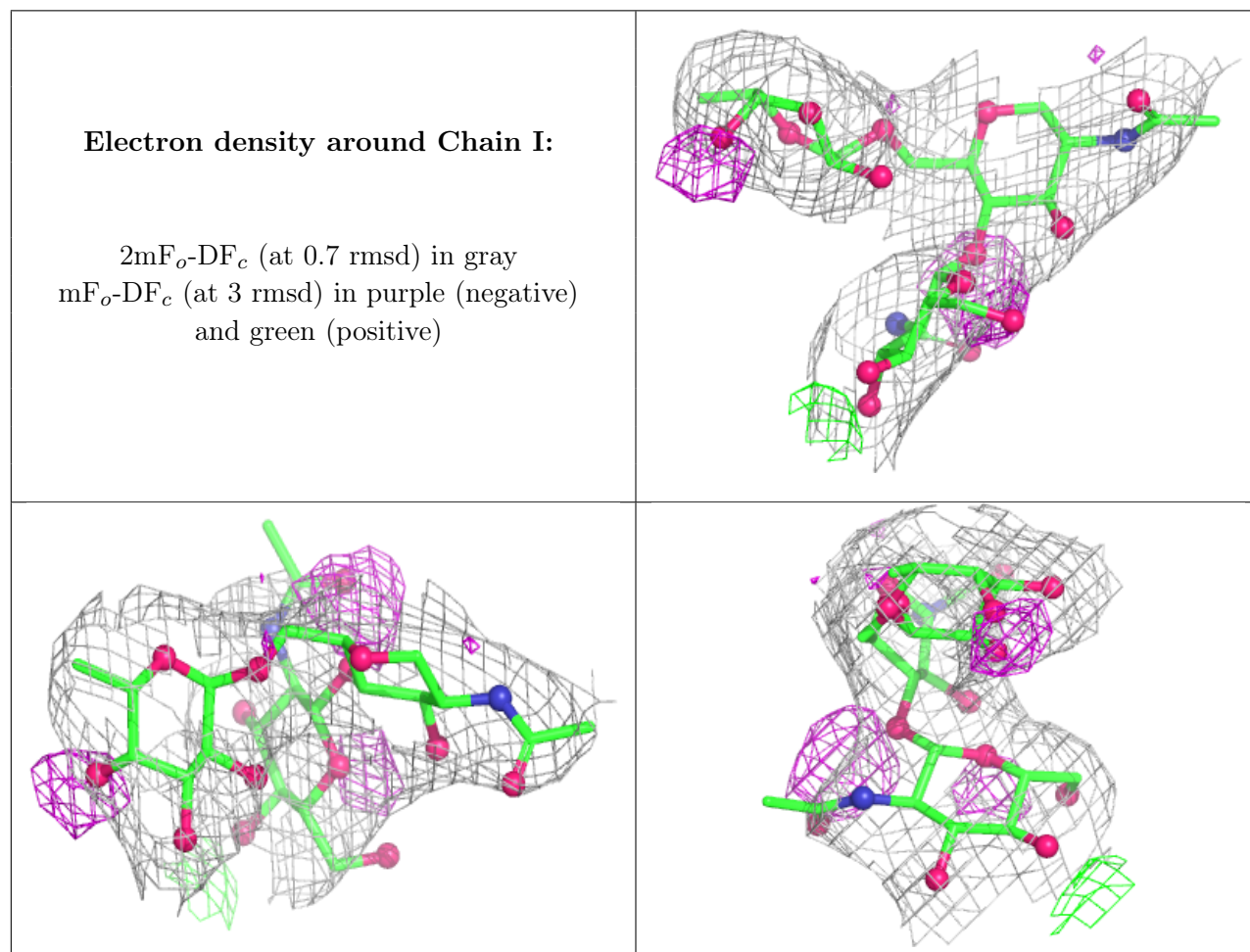
There are no non-standard protein/DNA/RNA residues in this entry.

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.

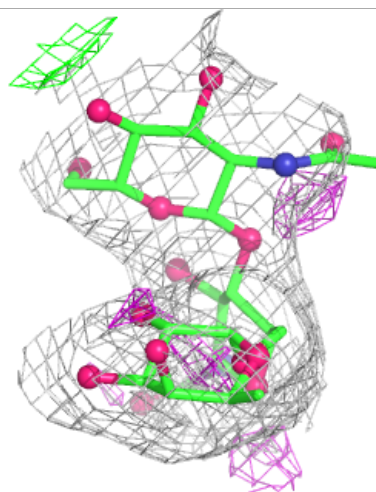
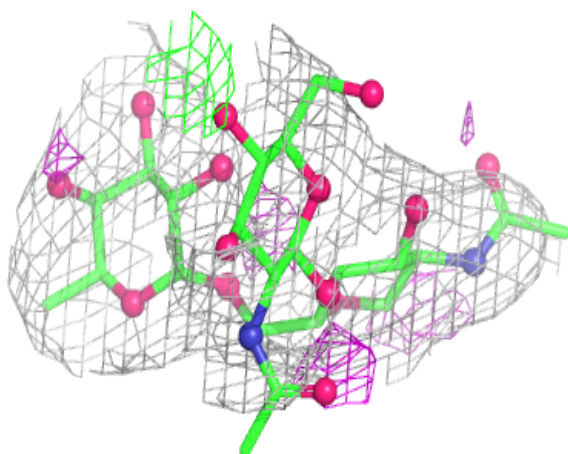
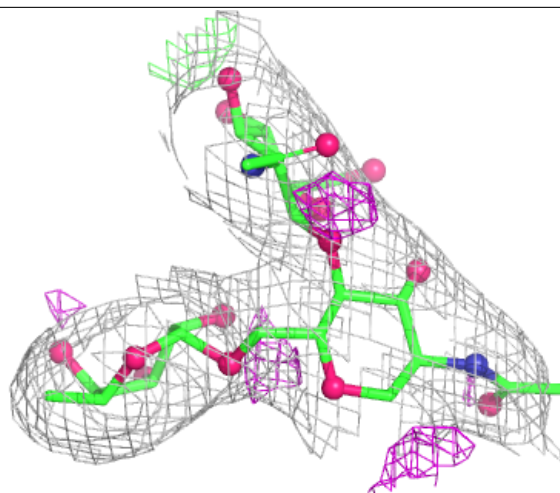
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FUC	L	3	10/11	0.67	0.12	61,88,102,106	0
3	FUC	K	3	10/11	0.70	0.11	64,86,104,108	0
3	FUC	I	3	10/11	0.73	0.12	56,84,98,100	0
3	NAG	K	2	14/15	0.74	0.12	83,94,98,98	0
3	NAG	J	2	14/15	0.75	0.13	84,103,121,126	0
3	NAG	L	2	14/15	0.77	0.12	87,98,105,108	0
3	NAG	I	2	14/15	0.79	0.13	83,98,114,118	0
3	FUC	J	3	10/11	0.79	0.12	57,77,84,88	0
3	NAG	L	1	14/15	0.94	0.08	66,77,88,91	0
3	NAG	J	1	14/15	0.94	0.09	61,69,86,93	0
3	NAG	K	1	14/15	0.94	0.07	60,70,85,86	0
3	NAG	I	1	14/15	0.96	0.07	60,64,83,83	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.



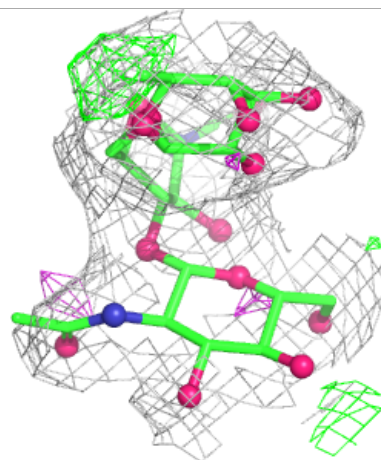
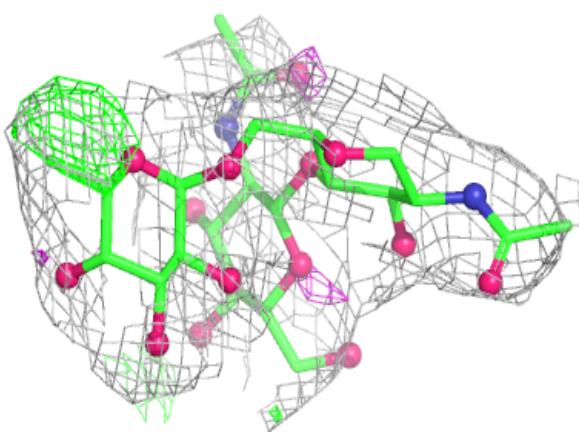
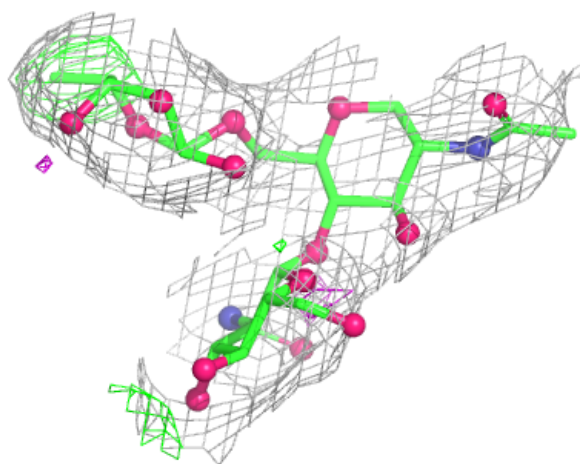
Electron density around Chain J:

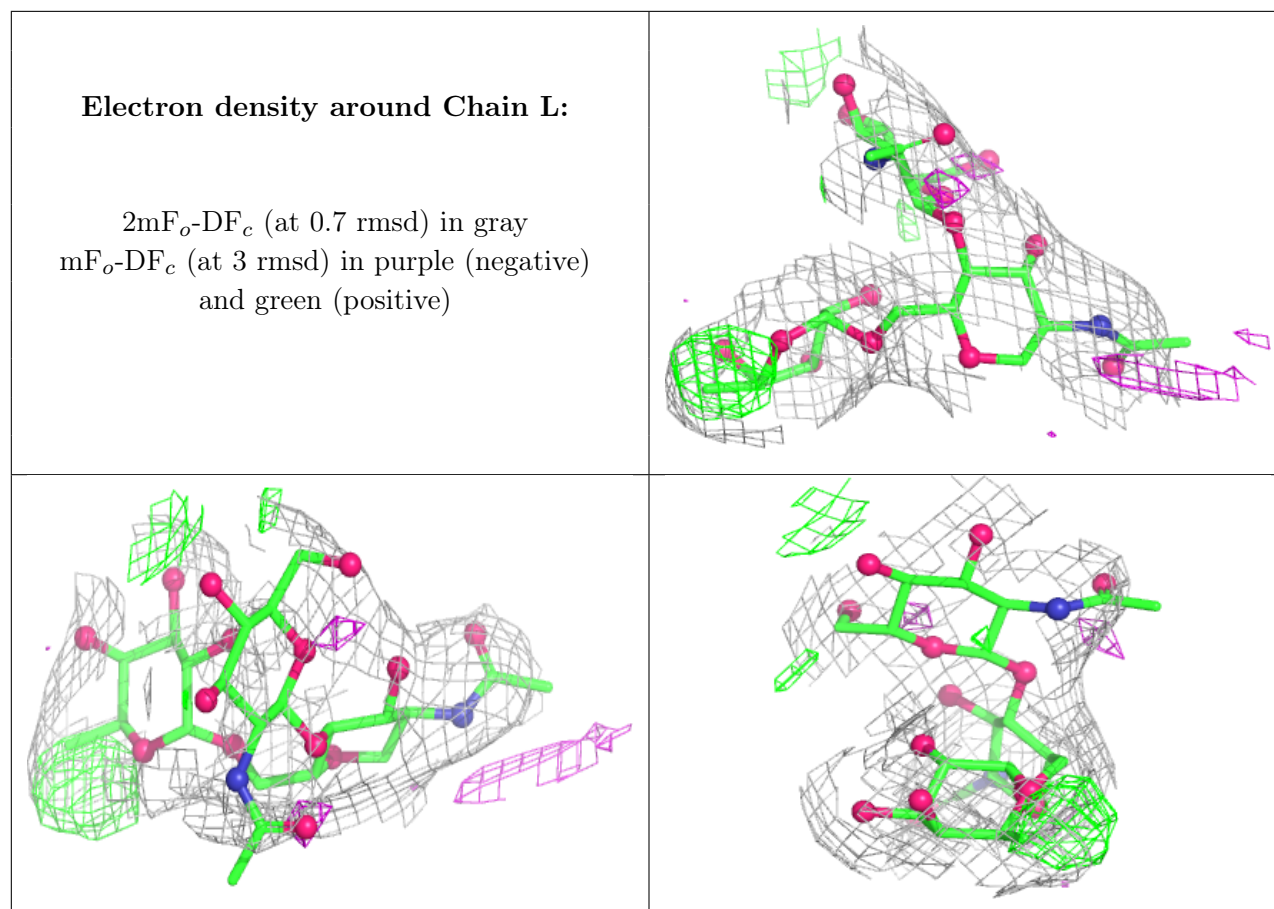
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain K:

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





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	E	1001	14/15	0.44	0.15	159,167,178,178	0
4	NAG	A	401	14/15	0.46	0.17	86,114,122,134	0
4	NAG	G	1000	14/15	0.47	0.17	92,130,132,135	0
4	NAG	C	401	14/15	0.48	0.20	100,126,136,154	0
4	NAG	C	402	14/15	0.48	0.14	142,158,164,166	0
4	NAG	A	402	14/15	0.52	0.14	140,161,166,168	0
4	NAG	E	1000	14/15	0.52	0.14	85,126,131,133	0
4	NAG	G	1001	14/15	0.60	0.12	147,164,177,179	0
4	NAG	C	403	14/15	0.66	0.13	158,173,188,188	0
4	NAG	A	403	14/15	0.68	0.13	155,167,177,177	0
4	NAG	G	1002	14/15	0.75	0.10	127,140,149,149	0
4	NAG	E	1002	14/15	0.83	0.09	132,142,155,157	0
6	CA	D	301	1/1	0.97	0.06	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CA	B	301	1/1	0.98	0.06	63,63,63,63	0
6	CA	F	301	1/1	0.98	0.04	85,85,85,85	0
6	CA	H	301	1/1	0.98	0.04	80,80,80,80	0
5	ZN	A	404	1/1	0.99	0.03	69,69,69,69	0
5	ZN	C	404	1/1	0.99	0.03	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.