



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 06:15 AM UTC

PDB ID : 3HUS / pdb_00003hus
Title : Crystal structure of recombinant gamma N308K fibrinogen fragment D with the peptide ligand Gly-Pro-Arg-Pro-amide
Authors : Lord, S.T.; Bowley, S.R.; Okumura, N.
Deposited on : 2009-06-15
Resolution : 3.04 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

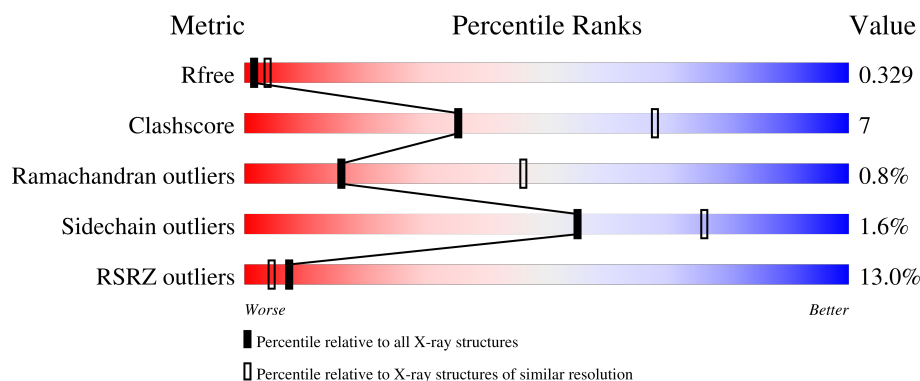
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 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	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

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	
1	D	66	
2	B	313	
2	E	313	
3	C	311	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	311	10% 78% 14% 6%
4	G	4	25% 100%
4	H	4	75% 75% 25%
4	I	4	100% 75% 25%
4	J	4	50% 50% 50%
5	K	3	67% 33%
5	L	3	33% 33% 33%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10837 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	61	Total	C	N	O	S	0	0	0
			497	305	95	94	3			
1	D	61	Total	C	N	O	S	0	0	0
			497	305	95	94	3			

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	303	Total	C	N	O	S	0	0	0
			2428	1514	429	463	22			
2	E	303	Total	C	N	O	S	0	0	0
			2428	1514	429	463	22			

- Molecule 3 is a protein called Fibrinogen gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	291	Total	C	N	O	S	0	0	0
			2335	1483	393	448	11			
3	F	293	Total	C	N	O	S	0	0	0
			2352	1493	397	451	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	308	LYS	ASN	engineered mutation	UNP P02679
F	308	LYS	ASN	engineered mutation	UNP P02679

- Molecule 4 is a protein called Peptide Ligand Gly-Pro-Arg-Pro-amide.

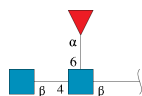
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			30	18	7	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	4	Total	C	N	O	0	0	0
			30	18	7	5			
4	I	4	Total	C	N	O	0	0	0
			30	18	7	5			
4	J	4	Total	C	N	O	0	0	0
			30	18	7	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 (CCD ID: 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	6	Total	O	0	0
			6	6		
7	B	26	Total	O	0	0
			26	26		
7	C	14	Total	O	0	0
			14	14		

Continued on next page...

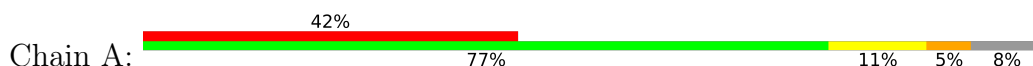
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	4	Total 4	O 4	0	0
7	E	33	Total 33	O 33	0	0
7	F	17	Total 17	O 17	0	0

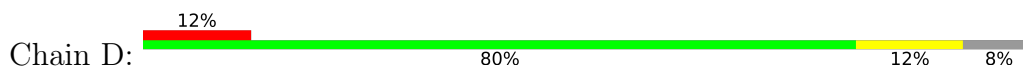
3 Residue-property plots [i](#)

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.

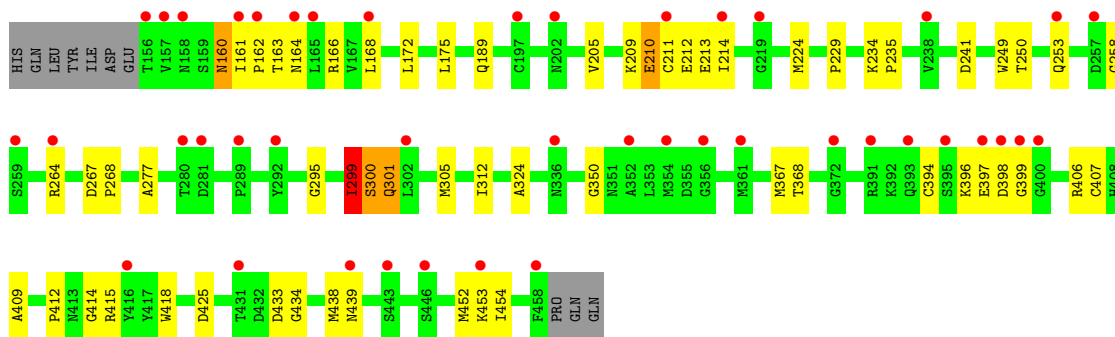
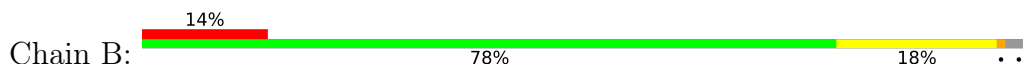
- Molecule 1: Fibrinogen alpha chain



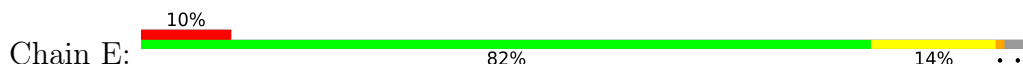
- Molecule 1: Fibrinogen alpha chain



- Molecule 2: Fibrinogen beta chain

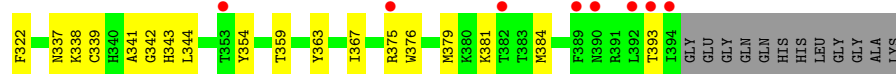
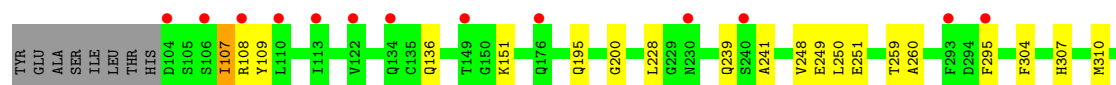
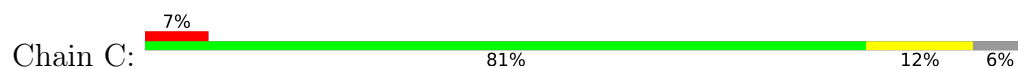


- Molecule 2: Fibrinogen beta chain

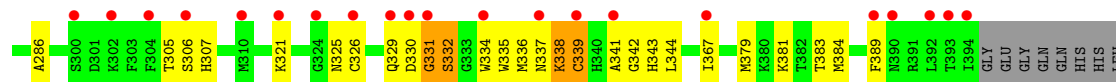
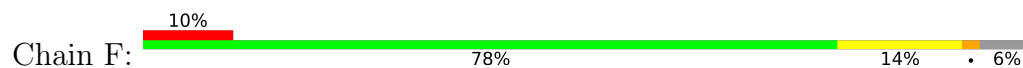




- Molecule 3: Fibrinogen gamma chain



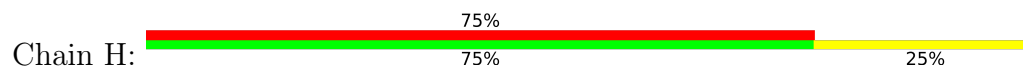
- Molecule 3: Fibrinogen gamma chain



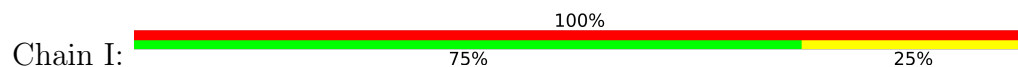
- Molecule 4: Peptide Ligand Gly-Pro-Arg-Pro-amide



- Molecule 4: Peptide Ligand Gly-Pro-Arg-Pro-amide



- Molecule 4: Peptide Ligand Gly-Pro-Arg-Pro-amide



- Molecule 4: Peptide Ligand Gly-Pro-Arg-Pro-amide



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	95.01Å 95.01Å 448.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.25 – 3.04 47.25 – 3.04	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.25-3.04) 99.3 (47.25-3.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.14 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.220 , 0.288 0.293 , 0.329	Depositor DCC
R_{free} test set	2030 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	65.0	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 30.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	10837	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9848e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CA, NAG, FUC

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	0.52	0/498	0.85	0/665
1	D	0.36	0/498	0.78	0/665
2	B	0.48	0/2489	0.73	1/3362 (0.0%)
2	E	0.50	0/2489	0.73	1/3362 (0.0%)
3	C	0.40	0/2399	0.68	0/3243
3	F	0.50	1/2417 (0.0%)	0.71	2/3268 (0.1%)
4	G	0.60	0/31	0.58	0/40
4	H	0.61	0/31	0.70	0/40
4	I	0.64	0/31	0.80	0/40
4	J	0.60	0/31	0.64	0/40
All	All	0.47	1/10914 (0.0%)	0.72	4/14725 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	197	ARG	CA-C	-7.13	1.44	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	198	LEU	CA-C-N	-7.49	108.49	120.70
3	F	198	LEU	C-N-CA	-7.49	108.49	120.70
2	B	299	ILE	CB-CA-C	-6.02	104.17	112.24
2	E	409	ALA	N-CA-C	-5.07	107.48	113.97

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	497	0	517	12	0
1	D	497	0	517	6	0
2	B	2428	0	2295	46	0
2	E	2428	0	2296	34	0
3	C	2335	0	2192	24	0
3	F	2352	0	2208	47	0
4	G	30	0	32	0	0
4	H	30	0	32	1	0
4	I	30	0	32	1	0
4	J	30	0	32	3	0
5	K	38	0	34	0	0
5	L	38	0	34	1	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	6	0	0	0	0
7	B	26	0	0	1	0
7	C	14	0	0	1	0
7	D	4	0	0	0	0
7	E	33	0	0	2	0
7	F	17	0	0	0	0
All	All	10837	0	10221	154	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 7.

All (154) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ARG:NH1	2:B:418:TRP:CE3	2.08	1.22
3:F:198:LEU:HD12	3:F:198:LEU:N	1.50	1.17
3:F:326:CYS:HB3	3:F:339:CYS:SG	1.85	1.16
3:F:326:CYS:CB	3:F:339:CYS:SG	2.41	1.08
1:A:159:ARG:O	2:B:258:GLY:O	1.70	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:338:LYS:NZ	4:I:3:ARG:O	1.97	0.96
2:E:397:GLU:HG2	2:E:431:THR:HG21	1.52	0.90
3:F:198:LEU:HD12	3:F:198:LEU:H	1.15	0.90
3:F:338:LYS:H	3:F:339:CYS:HA	1.37	0.88
3:F:338:LYS:O	3:F:338:LYS:HG3	1.75	0.86
3:F:338:LYS:N	3:F:339:CYS:HA	1.89	0.86
3:F:331:GLY:O	3:F:332:SER:HB3	1.77	0.83
2:E:378:TYR:HB2	2:E:396:LYS:HG3	1.62	0.82
3:C:200:GLY:HA2	7:C:83:HOH:O	1.81	0.80
3:F:198:LEU:N	3:F:198:LEU:CD1	2.30	0.78
3:F:338:LYS:H	3:F:339:CYS:CA	1.96	0.77
2:E:395:SER:O	2:E:396:LYS:HB2	1.84	0.76
2:B:160:ASN:O	2:B:162:PRO:HD3	1.85	0.76
3:F:336:MET:HE1	3:F:343:HIS:NE2	2.02	0.74
4:J:3:ARG:HH11	4:J:3:ARG:HG3	1.53	0.73
3:F:338:LYS:O	3:F:338:LYS:CG	2.36	0.72
2:B:295:GLY:O	2:B:299:ILE:HG13	1.89	0.71
2:B:399:GLY:HA3	2:B:414:GLY:HA2	1.73	0.69
2:B:264:ARG:HH21	3:C:136:GLN:HA	1.59	0.67
3:F:337:ASN:O	3:F:338:LYS:CB	2.42	0.67
1:A:154:ILE:O	1:A:158:ILE:HG13	1.95	0.66
3:C:251:GLU:HB3	3:C:381:LYS:HB2	1.79	0.65
3:F:307:HIS:HE1	3:F:342:GLY:H	1.43	0.65
2:B:253:GLN:HE22	2:B:412:PRO:HB2	1.62	0.65
2:B:301:GLN:NE2	2:B:305:MET:SD	2.69	0.64
3:F:326:CYS:CB	3:F:339:CYS:HG	2.00	0.63
2:B:300:SER:O	2:B:301:GLN:C	2.37	0.63
2:E:397:GLU:HG2	2:E:431:THR:CG2	2.26	0.63
2:B:209:LYS:C	2:B:210:GLU:HG3	2.23	0.62
2:E:453:LYS:NZ	7:E:50:HOH:O	2.31	0.62
1:A:158:ILE:HG23	2:B:189:GLN:HE21	1.64	0.62
3:F:334:TRP:O	3:F:336:MET:N	2.30	0.62
2:B:396:LYS:O	2:B:397:GLU:HG2	2.00	0.61
3:C:307:HIS:HE1	3:C:342:GLY:H	1.48	0.61
3:F:338:LYS:N	3:F:339:CYS:CA	2.60	0.60
3:F:196:LYS:O	3:F:197:ARG:HG2	2.01	0.60
3:F:251:GLU:HB3	3:F:381:LYS:HB2	1.84	0.60
2:B:209:LYS:HG3	2:B:213:GLU:OE2	2.02	0.59
2:B:367:MET:HB2	2:B:406:ARG:HB2	1.82	0.59
2:B:438:MET:HE1	4:H:1:GLY:HA2	1.83	0.59
3:F:344:LEU:HA	3:F:367:ILE:HG23	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:398:ASP:HA	2:B:433:ASP:HB3	1.85	0.59
3:F:336:MET:HE1	3:F:343:HIS:CD2	2.39	0.58
3:F:196:LYS:O	3:F:197:ARG:CG	2.52	0.58
3:F:151:LYS:HB3	3:F:239:GLN:HE22	1.68	0.57
2:E:364:ASN:HD21	5:L:1:NAG:H2	1.70	0.57
3:F:305:THR:HB	3:F:341:ALA:HB2	1.86	0.57
2:E:438:MET:HE1	4:J:1:GLY:HA2	1.87	0.56
2:E:253:GLN:HE22	2:E:412:PRO:HB2	1.70	0.55
3:C:304:PHE:HB3	3:C:338:LYS:HB3	1.88	0.55
1:A:158:ILE:HG23	2:B:189:GLN:HG3	1.89	0.54
3:F:245:ALA:HB2	3:F:389:PHE:HD1	1.71	0.54
2:E:428:LYS:O	2:E:428:LYS:HG3	2.08	0.54
1:A:158:ILE:CG2	2:B:189:GLN:HE21	2.21	0.54
2:B:164:ASN:O	2:B:168:LEU:HB2	2.09	0.53
1:A:159:ARG:C	1:A:160:SER:OG	2.50	0.53
2:E:428:LYS:O	2:E:428:LYS:CG	2.52	0.52
2:E:249:TRP:HB3	2:E:453:LYS:HB3	1.91	0.52
4:J:3:ARG:HG3	4:J:3:ARG:NH1	2.19	0.52
1:A:149:ARG:HH21	2:B:425:ASP:HA	1.75	0.52
2:E:157:VAL:HG22	2:E:158:ASN:H	1.74	0.51
3:F:306:SER:O	3:F:337:ASN:ND2	2.27	0.51
1:D:137:GLN:HE21	1:D:188:VAL:HG12	1.75	0.50
2:B:209:LYS:CG	2:B:213:GLU:OE2	2.59	0.50
3:C:195:GLN:HB3	3:C:384:MET:HB2	1.94	0.50
3:C:338:LYS:N	3:C:339:CYS:HA	2.25	0.49
1:A:159:ARG:NH1	2:B:418:TRP:CZ3	2.69	0.49
1:A:159:ARG:O	1:A:160:SER:OG	2.30	0.49
3:F:325:ASN:O	3:F:329:GLN:HG2	2.13	0.49
2:B:312:ILE:HB	2:B:324:ALA:HB3	1.95	0.49
2:E:389:ASP:HB3	2:E:392:LYS:HB2	1.95	0.49
2:B:211:CYS:HA	2:B:214:ILE:HD12	1.95	0.48
2:B:209:LYS:CD	2:B:213:GLU:OE2	2.61	0.48
2:B:350:GLY:HA3	2:B:439:ASN:HB3	1.95	0.48
3:F:111:GLN:HA	3:F:114:TYR:HB3	1.95	0.48
3:F:183:GLU:HB3	3:F:191:TRP:HB2	1.94	0.48
3:C:107:ILE:C	3:C:109:TYR:H	2.22	0.48
2:E:176:ARG:HE	3:F:113:ILE:HD11	1.78	0.48
2:B:295:GLY:O	2:B:299:ILE:CG1	2.61	0.48
2:E:398:ASP:HA	2:E:433:ASP:HB3	1.95	0.48
3:F:337:ASN:O	3:F:338:LYS:HB3	2.12	0.48
2:E:250:THR:HB	2:E:454:ILE:HG13	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:415:ARG:O	2:B:434:GLY:HA2	2.14	0.47
2:E:397:GLU:O	2:E:431:THR:OG1	2.32	0.47
3:F:321:LYS:HB2	3:F:337:ASN:O	2.14	0.47
2:B:267:ASP:HB3	2:B:268:PRO:HD3	1.97	0.47
2:B:368:THR:HB	2:B:409:ALA:HB2	1.96	0.47
2:E:298:LYS:HA	7:E:60:HOH:O	2.14	0.46
2:E:373:MET:HE2	2:E:405:ASN:HA	1.97	0.46
3:C:249:GLU:HG2	3:C:259:THR:HG22	1.97	0.46
2:E:428:LYS:HG2	2:E:429:HIS:CD2	2.51	0.46
3:C:310:MET:HE2	3:C:337:ASN:HA	1.98	0.46
2:E:161:ILE:O	2:E:164:ASN:HB3	2.14	0.46
2:B:241:ASP:HB3	2:B:249:TRP:HB2	1.97	0.46
3:F:250:LEU:HD22	3:F:379:MET:HG3	1.97	0.46
2:B:249:TRP:HB3	2:B:453:LYS:HB2	1.98	0.45
3:F:337:ASN:O	3:F:338:LYS:HB2	2.16	0.45
2:B:209:LYS:HE3	2:B:305:MET:HE1	1.99	0.45
2:B:210:GLU:OE2	2:B:212:GLU:HB3	2.17	0.45
1:D:150:LEU:HD21	3:F:124:LEU:HD23	1.99	0.45
2:E:406:ARG:N	2:E:407:CYS:HA	2.31	0.45
2:E:406:ARG:O	2:E:406:ARG:CG	2.63	0.45
3:C:307:HIS:CE1	3:C:341:ALA:H	2.35	0.44
1:D:139:ASN:HB3	3:F:114:TYR:CZ	2.52	0.44
2:E:415:ARG:O	2:E:434:GLY:HA2	2.17	0.44
3:F:331:GLY:O	3:F:332:SER:CB	2.54	0.44
2:B:396:LYS:C	2:B:398:ASP:H	2.25	0.44
3:C:307:HIS:HE1	3:C:341:ALA:H	1.65	0.44
2:E:230:ASP:HB2	2:E:233:VAL:HG22	1.99	0.44
3:C:248:VAL:HB	3:C:260:ALA:HB3	1.99	0.44
3:C:344:LEU:HA	3:C:367:ILE:HG23	1.99	0.43
3:C:107:ILE:HG22	3:C:108:ARG:H	1.82	0.43
2:B:205:VAL:HG11	3:C:228:LEU:HA	1.99	0.43
2:E:205:VAL:HG21	3:F:226:PHE:HB2	2.00	0.43
2:B:253:GLN:HB3	2:B:452:MET:HB2	2.01	0.43
2:E:357:ALA:HB3	2:E:360:LEU:HD12	1.99	0.43
3:C:359:THR:HG21	3:C:363:TYR:O	2.18	0.43
2:E:350:GLY:HA3	2:E:439:ASN:HB3	2.01	0.42
2:E:406:ARG:O	2:E:406:ARG:HG2	2.19	0.42
3:F:326:CYS:O	3:F:330:ASP:HB2	2.19	0.42
2:B:250:THR:HB	2:B:454:ILE:HG13	2.00	0.42
2:E:224:MET:HE3	2:E:277:ALA:HB3	2.01	0.42
1:A:147:MET:HG3	2:B:175:LEU:HD22	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:260:ALA:HB2	3:F:286:ALA:HB3	2.02	0.42
3:F:248:VAL:HB	3:F:260:ALA:HB3	2.01	0.42
2:B:394:CYS:O	2:B:398:ASP:HB2	2.19	0.42
2:B:406:ARG:N	2:B:407:CYS:HA	2.35	0.42
3:C:151:LYS:HB3	3:C:239:GLN:HE22	1.84	0.42
3:C:343:HIS:O	3:C:367:ILE:HA	2.18	0.42
3:F:195:GLN:HB3	3:F:384:MET:HB2	2.02	0.42
2:B:163:THR:HG22	2:B:166:ARG:NH2	2.35	0.41
2:B:163:THR:HG22	2:B:166:ARG:HH21	1.85	0.41
2:E:395:SER:O	2:E:396:LYS:CB	2.63	0.41
3:C:307:HIS:CE1	3:C:342:GLY:H	2.34	0.41
3:C:295:PHE:HB3	3:C:375:ARG:HH21	1.84	0.41
3:C:322:PHE:HD1	3:C:338:LYS:HE2	1.85	0.41
3:C:354:TYR:O	3:C:376:TRP:HB3	2.20	0.41
1:A:161:CYS:HA	1:A:164:SER:HB2	2.01	0.41
2:B:224:MET:HE3	2:B:277:ALA:HB3	2.02	0.41
3:C:250:LEU:HD22	3:C:379:MET:HG3	2.02	0.41
1:D:169:LEU:H	2:E:189:GLN:HE22	1.69	0.41
3:F:196:LYS:C	3:F:197:ARG:CG	2.93	0.41
1:D:147:MET:HG3	2:E:175:LEU:HD22	2.01	0.41
3:F:166:LEU:HD13	3:F:179:LEU:HD21	2.02	0.41
3:F:249:GLU:HB3	3:F:383:THR:HB	2.03	0.41
2:B:229:PRO:HG2	7:B:81:HOH:O	2.21	0.40
2:B:234:LYS:HA	2:B:235:PRO:HD3	1.99	0.40
1:D:136:LEU:HD21	3:F:111:GLN:HB3	2.02	0.40
2:E:303:THR:HB	2:E:330:THR:HA	2.02	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	59/66 (89%)	55 (93%)	3 (5%)	1 (2%)	7	29
1	D	59/66 (89%)	58 (98%)	1 (2%)	0	100	100
2	B	301/313 (96%)	271 (90%)	29 (10%)	1 (0%)	36	67
2	E	301/313 (96%)	275 (91%)	24 (8%)	2 (1%)	18	49
3	C	289/311 (93%)	267 (92%)	21 (7%)	1 (0%)	36	67
3	F	291/311 (94%)	265 (91%)	21 (7%)	5 (2%)	7	29
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	1308/1396 (94%)	1199 (92%)	99 (8%)	10 (1%)	16	46

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	157	VAL
3	F	335	TRP
3	F	338	LYS
1	A	160	SER
2	E	396	LYS
3	F	331	GLY
3	F	332	SER
3	C	241	ALA
3	F	241	ALA
2	B	160	ASN

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	56/61 (92%)	52 (93%)	4 (7%)	13	40
1	D	56/61 (92%)	55 (98%)	1 (2%)	51	74

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	261/271 (96%)	255 (98%)	6 (2%)	44	70
2	E	261/271 (96%)	259 (99%)	2 (1%)	73	83
3	C	245/259 (95%)	243 (99%)	2 (1%)	73	83
3	F	247/259 (95%)	244 (99%)	3 (1%)	63	79
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	1138/1194 (95%)	1120 (98%)	18 (2%)	55	76

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	LEU
1	A	158	ILE
1	A	159	ARG
1	A	176	LYS
2	B	161	ILE
2	B	172	LEU
2	B	210	GLU
2	B	299	ILE
2	B	300	SER
2	B	301	GLN
3	C	107	ILE
3	C	393	THR
1	D	173	VAL
2	E	280	THR
2	E	428	LYS
3	F	143	VAL
3	F	198	LEU
3	F	339	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	HIS
1	A	181	GLN
2	B	174	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	189	GLN
2	B	202	ASN
2	B	253	GLN
2	B	254	ASN
2	B	336	ASN
2	B	339	GLN
2	B	408	HIS
3	C	111	GLN
3	C	136	GLN
3	C	146	HIS
3	C	176	GLN
3	C	177	GLN
3	C	189	ASN
3	C	230	ASN
3	C	239	GLN
3	C	307	HIS
3	C	319	ASN
2	E	174	ASN
2	E	189	GLN
2	E	228	GLN
2	E	253	GLN
2	E	256	GLN
2	E	301	GLN
2	E	339	GLN
2	E	364	ASN
2	E	408	HIS
3	F	103	HIS
3	F	115	ASN
3	F	117	ASN
3	F	119	GLN
3	F	123	ASN
3	F	136	GLN
3	F	146	HIS
3	F	230	ASN
3	F	239	GLN
3	F	307	HIS
3	F	317	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	0.51	0	17,19,21	0.81	0
5	NAG	K	2	5	14,14,15	0.78	0	17,19,21	2.51	6 (35%)
5	FUC	K	3	5	10,10,11	0.63	0	14,14,16	0.63	0
5	NAG	L	1	5	14,14,15	0.55	0	17,19,21	0.96	1 (5%)
5	NAG	L	2	5	14,14,15	0.64	0	17,19,21	1.55	2 (11%)
5	FUC	L	3	5	10,10,11	0.61	0	14,14,16	0.67	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	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	5/6/23/26	0/1/1/1
5	FUC	K	3	5	-	-	0/1/1/1
5	NAG	L	1	5	-	2/6/23/26	0/1/1/1
5	NAG	L	2	5	-	4/6/23/26	0/1/1/1
5	FUC	L	3	5	-	-	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	2	NAG	C2-N2-C7	7.28	132.66	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	2	NAG	C4-C3-C2	4.28	117.29	111.02
5	L	2	NAG	C2-N2-C7	3.88	128.10	122.90
5	K	2	NAG	C8-C7-N2	3.67	122.21	116.12
5	L	2	NAG	C4-C3-C2	3.26	115.80	111.02
5	K	2	NAG	O7-C7-C8	-2.49	117.62	122.05
5	K	2	NAG	C3-C4-C5	2.40	114.59	110.23
5	K	2	NAG	C1-C2-N2	2.07	113.69	110.43
5	L	1	NAG	O5-C1-C2	-2.04	108.14	111.29

There are no chirality outliers.

All (11) torsion outliers are listed below:

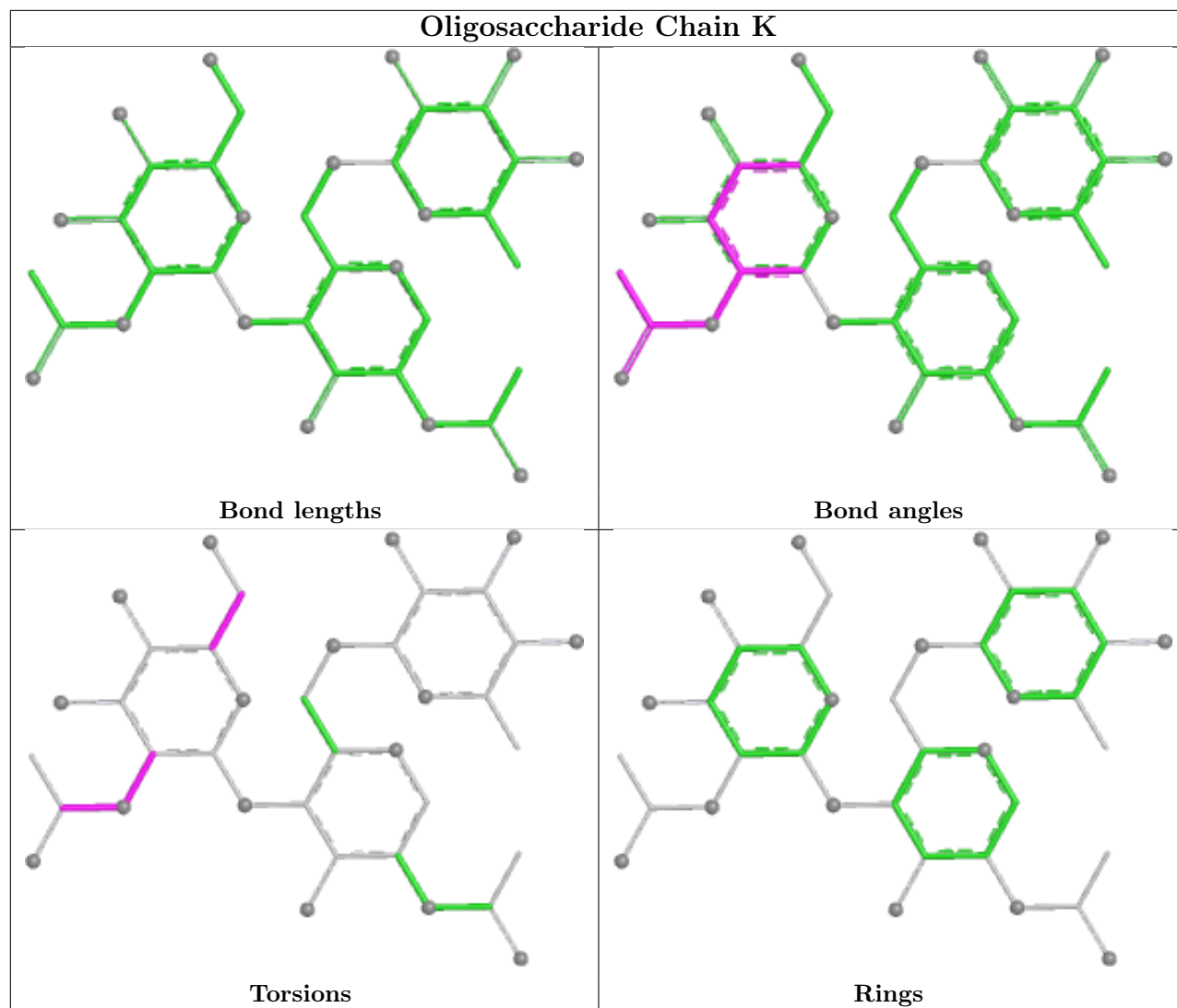
Mol	Chain	Res	Type	Atoms
5	L	1	NAG	O5-C5-C6-O6
5	L	1	NAG	C4-C5-C6-O6
5	K	2	NAG	C8-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2
5	K	2	NAG	C1-C2-N2-C7
5	L	2	NAG	C1-C2-N2-C7
5	L	2	NAG	C4-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
5	L	2	NAG	C3-C2-N2-C7
5	L	2	NAG	O5-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6

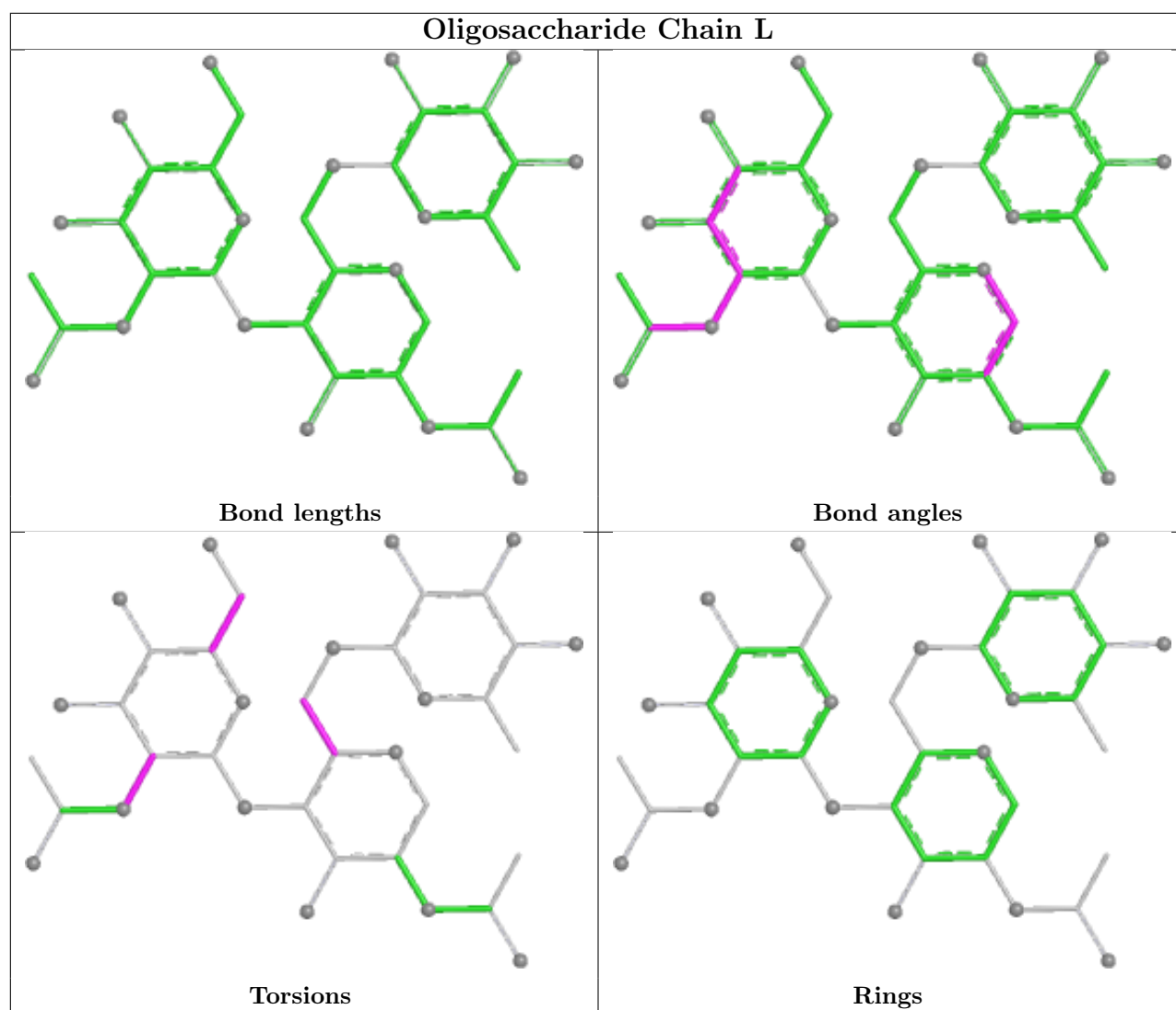
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	1	NAG	1	0

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





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	61/66 (92%)	2.13	28 (45%) 0 0	72, 87, 102, 102	0
1	D	61/66 (92%)	1.26	8 (13%) 7 4	60, 67, 78, 78	0
2	B	303/313 (96%)	1.18	43 (14%) 6 4	49, 58, 75, 88	0
2	E	303/313 (96%)	0.99	31 (10%) 12 6	46, 55, 68, 81	0
3	C	291/311 (93%)	0.90	21 (7%) 21 10	50, 59, 72, 83	0
3	F	293/311 (94%)	0.92	31 (10%) 11 6	50, 61, 73, 87	0
4	G	4/4 (100%)	1.41	1 (25%) 2 1	85, 85, 86, 86	0
4	H	4/4 (100%)	2.91	3 (75%) 0 0	88, 88, 88, 89	0
4	I	4/4 (100%)	2.51	4 (100%) 0 0	95, 95, 96, 96	0
4	J	4/4 (100%)	2.23	2 (50%) 0 0	78, 78, 78, 80	0
All	All	1328/1396 (95%)	1.08	172 (12%) 7 4	46, 59, 82, 102	0

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	395	SER	7.8
2	B	157	VAL	5.6
3	F	394	ILE	5.5
4	H	1	GLY	5.0
2	B	397	GLU	4.9
2	B	164	ASN	4.8
2	E	210	GLU	4.8
1	A	170	ALA	4.8
3	C	240	SER	4.8
1	D	164	SER	4.7
1	A	168	ALA	4.4
2	E	398	ASP	4.3
1	A	164	SER	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	394	ILE	4.3
1	A	162	ARG	4.2
2	E	163	THR	4.2
2	E	230	ASP	4.1
1	A	189	ILE	4.1
1	A	160	SER	4.1
3	F	392	LEU	3.9
1	A	169	LEU	3.9
1	A	130	VAL	3.8
3	F	326	CYS	3.8
1	D	168	ALA	3.7
2	E	305	MET	3.7
4	J	1	GLY	3.7
2	E	281	ASP	3.6
2	B	280	THR	3.6
2	B	458	PHE	3.6
3	F	337	ASN	3.6
2	E	393	GLN	3.5
2	E	396	LYS	3.5
1	A	190	ALA	3.5
2	B	156	THR	3.4
2	B	399	GLY	3.4
1	A	166	SER	3.4
3	C	106	SER	3.4
2	B	161	ILE	3.4
1	A	161	CYS	3.3
4	I	1	GLY	3.3
1	A	163	GLY	3.3
1	A	159	ARG	3.3
2	B	219	GLY	3.2
2	B	253	GLN	3.2
2	E	253	GLN	3.2
3	F	393	THR	3.2
1	A	131	GLN	3.2
2	E	376	SER	3.1
3	F	390	ASN	3.1
1	A	186	GLU	3.1
2	B	391	ARG	3.1
2	B	354	MET	3.1
2	B	443	SER	3.1
3	F	330	ASP	3.1
1	A	167	ARG	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	165	LEU	3.0
3	C	230	ASN	3.0
2	E	157	VAL	3.0
3	C	393	THR	3.0
1	D	169	LEU	2.9
1	D	163	GLY	2.9
2	B	398	ASP	2.9
3	F	102	THR	2.9
3	C	390	ASN	2.9
2	B	257	ASP	2.8
2	B	211	CYS	2.8
2	B	400	GLY	2.8
1	A	184	GLN	2.8
1	A	188	VAL	2.8
2	E	385	TRP	2.8
3	C	134	GLN	2.8
1	A	185	LEU	2.8
2	E	377	THR	2.8
2	E	378	TYR	2.7
1	D	167	ARG	2.7
2	B	168	LEU	2.7
3	F	341	ALA	2.7
1	A	187	GLN	2.7
2	B	361	MET	2.7
3	C	113	ILE	2.7
4	H	4	PRO	2.7
4	I	2	PRO	2.7
3	C	293	PHE	2.7
2	B	202	ASN	2.7
1	A	171	ARG	2.6
2	B	439	ASN	2.6
2	B	302	LEU	2.6
3	C	110	LEU	2.6
2	E	224	MET	2.6
3	C	149	THR	2.6
1	A	156	ILE	2.5
3	F	339	CYS	2.5
2	B	395	SER	2.5
2	B	158	ASN	2.5
3	C	392	LEU	2.5
2	B	446	SER	2.5
2	E	383	ASP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	295	PHE	2.5
3	C	353	THR	2.5
2	B	453	LYS	2.5
1	A	135	LEU	2.5
3	F	304	PHE	2.4
2	E	162	PRO	2.4
2	B	356	GLY	2.4
1	D	170	ALA	2.4
2	E	361	MET	2.4
3	F	389	PHE	2.4
3	C	382	THR	2.4
1	A	142	ALA	2.4
3	F	113	ILE	2.4
2	B	431	THR	2.4
1	A	139	ASN	2.4
2	E	447	MET	2.4
2	B	393	GLN	2.4
3	C	389	PHE	2.4
1	D	160	SER	2.4
1	D	187	GLN	2.3
2	E	453	LYS	2.3
2	B	197	CYS	2.3
3	C	108	ARG	2.3
2	B	292	TYR	2.3
2	E	416	TYR	2.3
3	F	310	MET	2.3
2	B	289	PRO	2.3
2	E	372	GLY	2.3
3	C	176	GLN	2.3
2	B	264	ARG	2.3
2	E	458	PHE	2.3
2	E	373	MET	2.2
2	B	416	TYR	2.2
2	B	259	SER	2.2
3	F	329	GLN	2.2
1	A	165	CYS	2.2
2	E	258	GLY	2.2
3	F	334	TRP	2.2
4	G	1	GLY	2.2
2	B	352	ALA	2.2
3	F	331	GLY	2.2
2	E	386	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	131	LEU	2.1
3	F	266	LYS	2.1
4	J	4	PRO	2.1
3	F	164	SER	2.1
3	F	306	SER	2.1
2	B	336	ASN	2.1
2	B	214	ILE	2.1
3	F	321	LYS	2.1
2	E	336	ASN	2.1
3	F	205	LYS	2.1
2	E	203	ILE	2.1
3	C	375	ARG	2.1
3	F	216	GLY	2.1
3	F	300	SER	2.1
1	A	173	VAL	2.1
1	A	133	ILE	2.1
3	F	271	ALA	2.1
3	F	111	GLN	2.1
4	H	2	PRO	2.1
3	F	106	SER	2.0
4	I	3	ARG	2.0
2	B	372	GLY	2.0
3	F	324	GLY	2.0
2	B	162	PRO	2.0
2	E	397	GLU	2.0
3	F	302	LYS	2.0
2	E	158	ASN	2.0
2	B	281	ASP	2.0
3	C	104	ASP	2.0
4	I	4	PRO	2.0
2	B	238	VAL	2.0
3	C	122	VAL	2.0
3	F	367	ILE	2.0

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

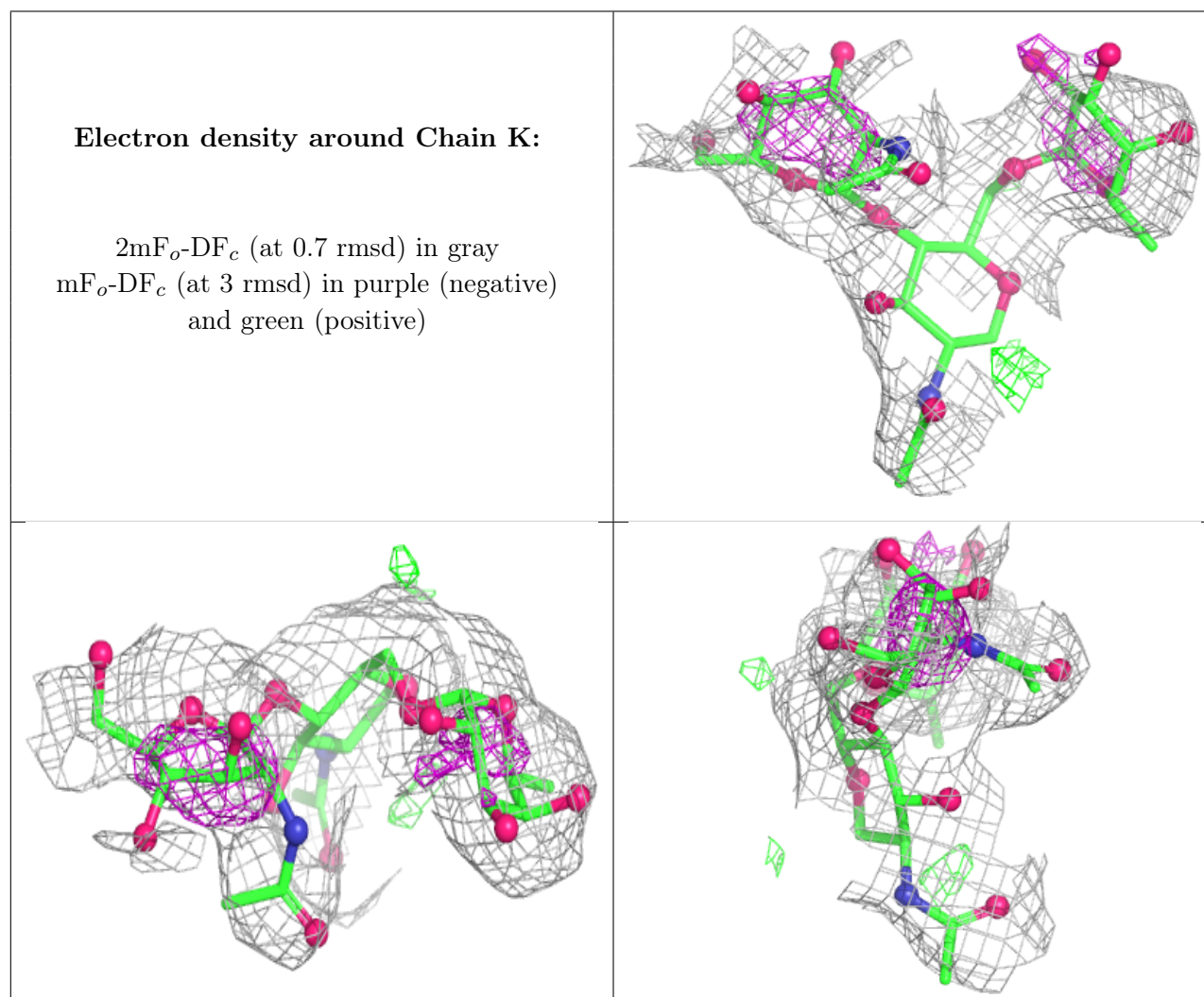
There are no non-standard protein/DNA/RNA residues in this entry.

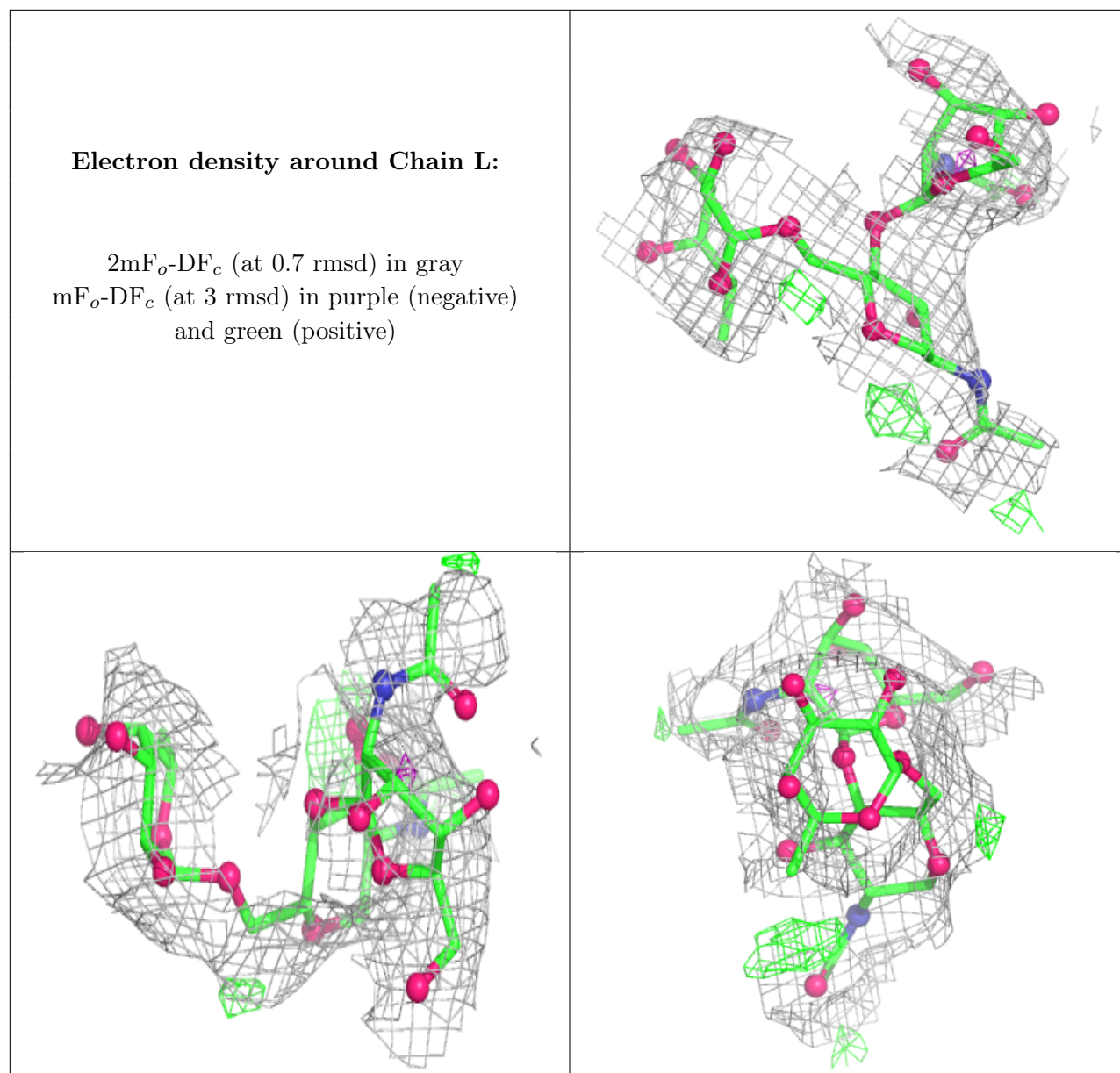
6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	K	2	14/15	0.25	0.18	100,101,102,102	0
5	NAG	L	2	14/15	0.48	0.18	134,135,135,135	0
5	FUC	L	3	10/11	0.49	0.17	135,135,135,135	0
5	NAG	K	1	14/15	0.52	0.17	89,92,97,97	0
5	FUC	K	3	10/11	0.53	0.20	99,99,100,100	0
5	NAG	L	1	14/15	0.55	0.20	132,134,135,135	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	C	1	1/1	0.35	0.17	68,68,68,68	0
6	CA	F	1	1/1	0.36	0.21	90,90,90,90	0
6	CA	B	2	1/1	0.43	0.22	69,69,69,69	0
6	CA	E	2	1/1	0.53	0.21	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.