



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:40 PM UTC

PDB ID : 4KI1 / pdb_00004ki1
Title : Primitive triclinic crystal form of the human IgE-Fc(epsilon)3-4 bound to its B cell receptor derCD23
Authors : Dhaliwal, B.; Pang, M.O.Y.; Sutton, B.J.; Beavil, A.J.
Deposited on : 2013-05-01
Resolution : 3.20 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

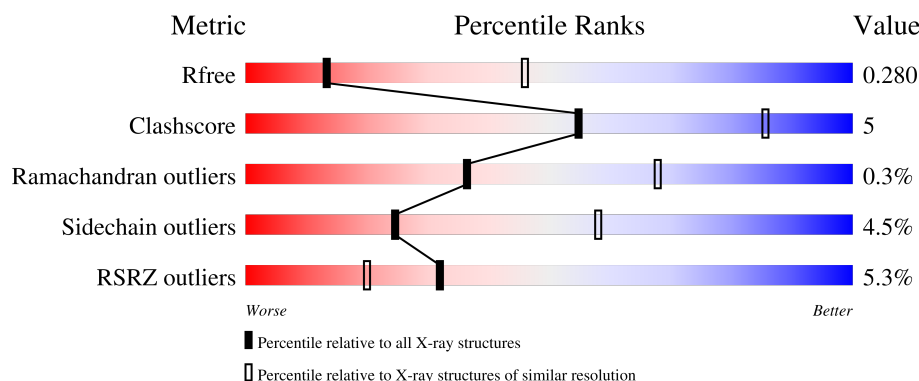
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	223	 4% 82% 10% • 7%
1	B	223	 4% 80% 13% • 5%
1	C	223	 3% 84% 9% • 5%
1	D	223	 2% 80% 12% • 7%
2	E	143	 6% 79% 13% • 8%

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Mol	Chain	Length	Quality of chain
2	F	143	13% 78% 13% 8%
2	G	143	6% 79% 13% 7%
2	H	143	6% 80% 12% 8%
3	I	5	40% 60%
3	J	5	40% 40% 20%
3	K	5	40% 20% 40%
3	L	5	20% 40% 40%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11133 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 IG EPSILON CHAIN C REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1650	1033	304	307	6			
1	B	211	Total	C	N	O	S	0	0	0
			1667	1044	307	310	6			
1	C	211	Total	C	N	O	S	0	0	0
			1667	1044	307	310	6			
1	D	208	Total	C	N	O	S	0	0	0
			1650	1033	304	307	6			

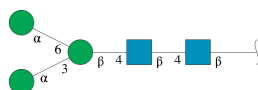
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	ALA	-	expression tag	UNP P01854
A	326	ASP	-	expression tag	UNP P01854
A	327	PRO	-	expression tag	UNP P01854
A	371	GLN	ASN	engineered mutation	UNP P01854
A	383	GLN	ASN	engineered mutation	UNP P01854
B	325	ALA	-	expression tag	UNP P01854
B	326	ASP	-	expression tag	UNP P01854
B	327	PRO	-	expression tag	UNP P01854
B	371	GLN	ASN	engineered mutation	UNP P01854
B	383	GLN	ASN	engineered mutation	UNP P01854
C	325	ALA	-	expression tag	UNP P01854
C	326	ASP	-	expression tag	UNP P01854
C	327	PRO	-	expression tag	UNP P01854
C	371	GLN	ASN	engineered mutation	UNP P01854
C	383	GLN	ASN	engineered mutation	UNP P01854
D	325	ALA	-	expression tag	UNP P01854
D	326	ASP	-	expression tag	UNP P01854
D	327	PRO	-	expression tag	UNP P01854
D	371	GLN	ASN	engineered mutation	UNP P01854
D	383	GLN	ASN	engineered mutation	UNP P01854

- Molecule 2 is a protein called LOW AFFINITY IMMUNOGLOBULIN EPSILON FC RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	132	Total	C	N	O	S	0	0	0
			1065	670	190	194	11			
2	F	131	Total	C	N	O	S	0	0	0
			1058	665	189	193	11			
2	G	133	Total	C	N	O	S	0	0	0
			1070	673	191	195	11			
2	H	132	Total	C	N	O	S	0	0	0
			1059	664	190	194	11			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	J	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	K	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	L	5	Total	C	N	O	0	0	0
			61	34	2	25			

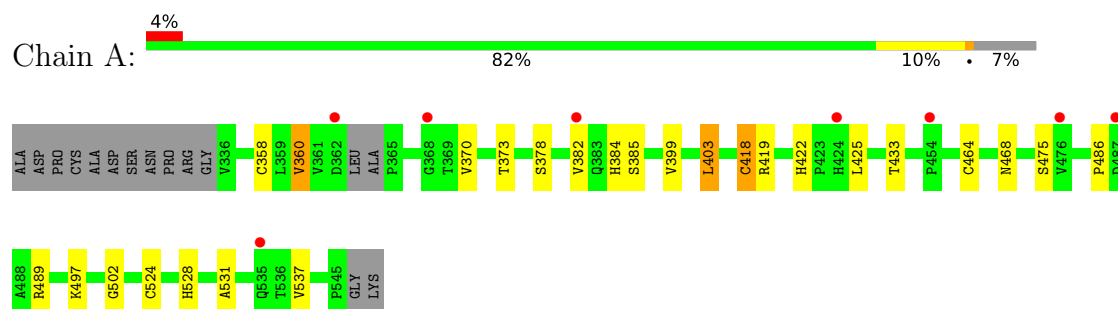
- Molecule 4 is water.

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

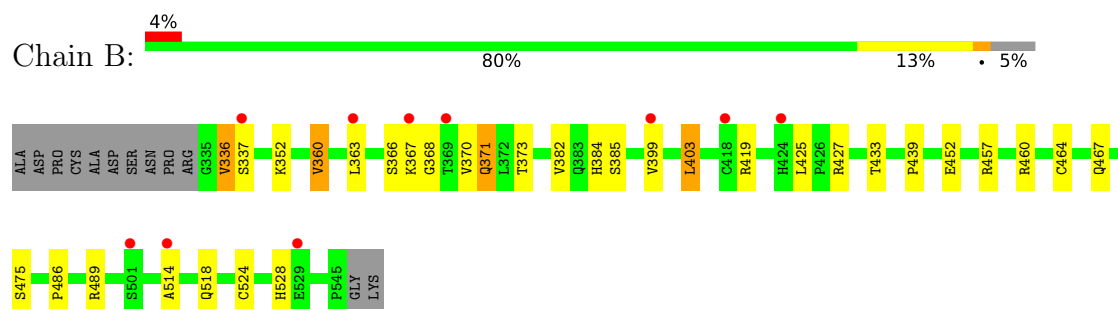
3 Residue-property plots

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.

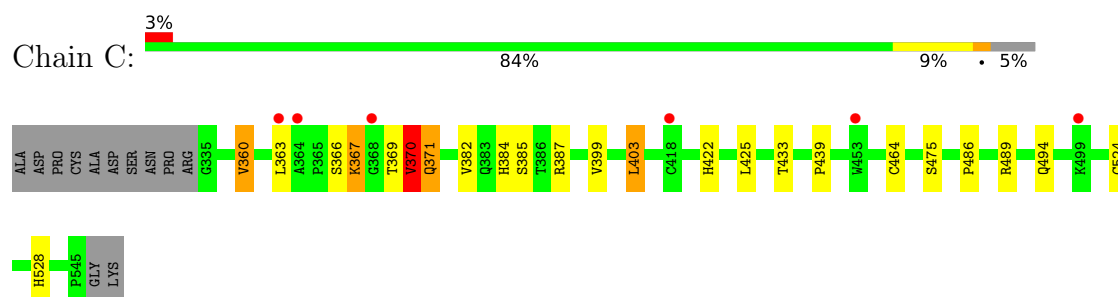
• Molecule 1: IG EPSILON CHAIN C REGION



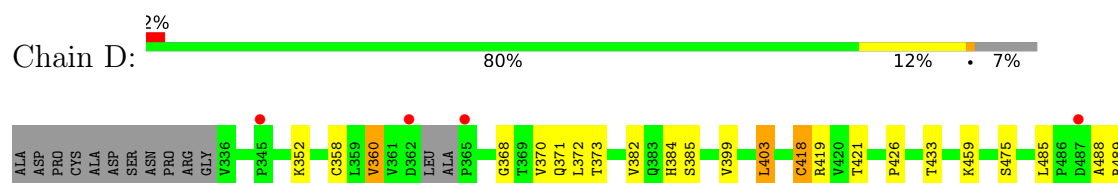
• Molecule 1: IG EPSILON CHAIN C REGION



• Molecule 1: IG EPSILON CHAIN C REGION

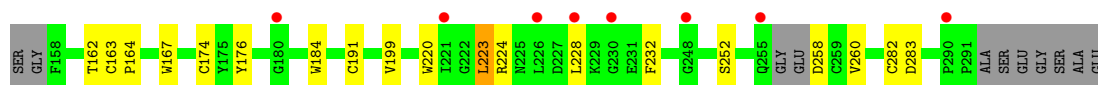
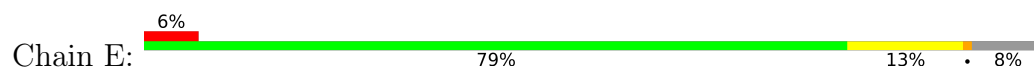


• Molecule 1: IG EPSILON CHAIN C REGION

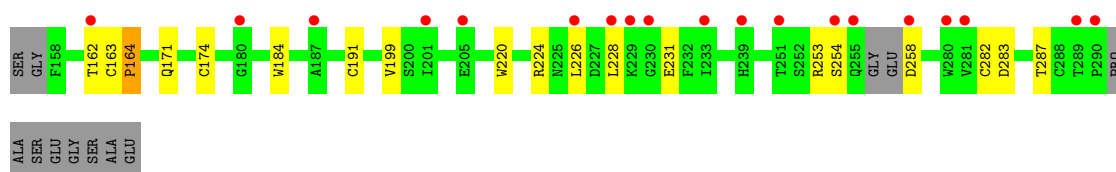
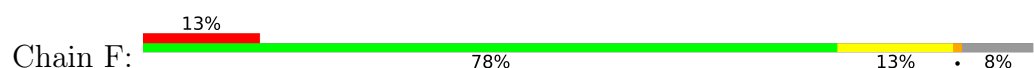




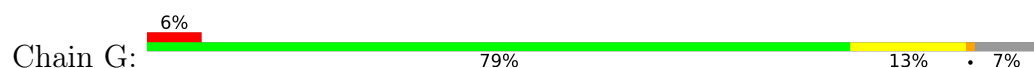
- Molecule 2: LOW AFFINITY IMMUNOGLOBULIN EPSILON FC RECEPTOR



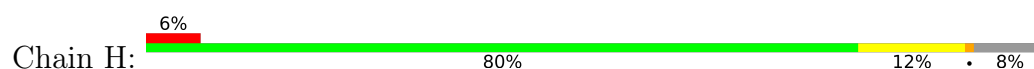
- Molecule 2: LOW AFFINITY IMMUNOGLOBULIN EPSILON FC RECEPTOR



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



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





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

Chain K:



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

Chain L:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	48.79Å 63.84Å 163.89Å 100.67° 90.13° 103.49°	Depositor
Resolution (Å)	80.40 – 3.20 80.40 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.8 (80.40-3.20) 96.8 (80.40-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 3.19Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.233 , 0.266 0.263 , 0.280	Depositor DCC
R_{free} test set	1523 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	58.7	Xtriage
Anisotropy	0.765	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.049 for -h,-k,k+1	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	11133	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.47% 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, MAN, BMA

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	0.67	0/1692	1.15	5/2301 (0.2%)
1	B	0.67	0/1710	1.16	6/2328 (0.3%)
1	C	0.71	0/1710	1.16	5/2328 (0.2%)
1	D	0.66	0/1692	1.20	9/2301 (0.4%)
2	E	0.72	1/1098 (0.1%)	1.23	1/1487 (0.1%)
2	F	0.71	1/1090 (0.1%)	1.24	2/1475 (0.1%)
2	G	0.78	2/1103 (0.2%)	1.31	6/1494 (0.4%)
2	H	0.72	1/1091 (0.1%)	1.23	1/1478 (0.1%)
All	All	0.70	5/11186 (0.0%)	1.20	35/15192 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	172	ARG	CA-C	8.83	1.64	1.53
2	E	164	PRO	N-CD	-6.80	1.38	1.47
2	G	164	PRO	N-CD	-6.01	1.39	1.47
2	F	164	PRO	N-CD	-6.00	1.39	1.47
2	H	164	PRO	N-CD	-5.78	1.39	1.47

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	384	HIS	N-CA-C	11.66	127.34	109.96
1	B	384	HIS	N-CA-C	11.49	127.08	109.96
1	D	384	HIS	N-CA-C	10.67	125.86	109.96
1	B	370	VAL	N-CA-C	10.37	121.19	110.72
1	C	384	HIS	N-CA-C	10.11	125.02	109.96
1	D	459	LYS	N-CA-C	9.38	124.62	108.76
2	G	173	LYS	N-CA-CB	6.88	122.37	111.43
1	D	488	ALA	N-CA-C	6.79	119.70	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	385	SER	N-CA-CB	6.55	121.09	110.41
1	B	385	SER	N-CA-CB	6.52	121.04	110.41
2	G	173	LYS	N-CA-C	-6.38	99.72	109.41
2	G	171	GLN	CB-CA-C	6.31	122.98	110.42
1	B	528	HIS	CA-C-N	6.11	128.75	120.38
1	B	528	HIS	C-N-CA	6.11	128.75	120.38
1	D	528	HIS	CA-C-N	6.09	128.73	120.38
1	D	528	HIS	C-N-CA	6.09	128.73	120.38
1	A	528	HIS	CA-C-N	5.97	128.56	120.38
1	A	528	HIS	C-N-CA	5.97	128.56	120.38
1	C	528	HIS	CA-C-N	5.89	128.45	120.38
1	C	528	HIS	C-N-CA	5.89	128.45	120.38
2	G	199	VAL	N-CA-C	5.87	116.98	109.30
2	E	199	VAL	N-CA-C	5.87	116.98	109.30
1	C	370	VAL	N-CA-C	5.84	116.58	110.62
2	F	199	VAL	N-CA-C	5.83	116.94	109.30
2	H	199	VAL	N-CA-C	5.76	116.84	109.30
1	D	418	CYS	N-CA-C	5.62	118.29	107.44
2	G	172	ARG	CA-C-O	5.59	128.10	121.17
1	C	385	SER	N-CA-CB	5.48	119.35	110.41
1	D	385	SER	N-CA-CB	5.41	119.23	110.41
1	D	490	HIS	N-CA-CB	5.41	120.33	111.08
1	A	418	CYS	N-CA-C	5.37	117.57	108.02
2	G	197	GLN	N-CA-C	5.30	117.74	109.52
1	D	426	PRO	N-CA-C	5.20	123.18	112.47
2	F	171	GLN	CB-CA-C	-5.08	110.73	116.63
1	B	467	GLN	N-CA-C	5.03	117.06	109.41

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	1650	0	1636	9	0
1	B	1667	0	1655	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1667	0	1655	13	0
1	D	1650	0	1636	9	0
2	E	1065	0	989	8	1
2	F	1058	0	982	11	0
2	G	1070	0	994	14	0
2	H	1059	0	985	10	1
3	I	61	0	52	0	0
3	J	61	0	52	1	0
3	K	61	0	52	2	0
3	L	61	0	52	1	0
4	B	2	0	0	0	0
4	D	1	0	0	0	0
All	All	11133	0	10740	88	1

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 5.

All (88) 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:F:163:CYS:SG	2:F:174:CYS:HB3	1.91	1.10
1:C:370:VAL:HG13	1:C:422:HIS:HD2	1.16	1.09
2:F:163:CYS:HB2	2:F:174:CYS:SG	2.05	0.96
2:G:163:CYS:SG	2:G:174:CYS:HB3	2.06	0.96
1:A:358:CYS:HG	1:A:418:CYS:HG	1.01	0.93
1:C:464:CYS:HG	1:C:524:CYS:HG	0.94	0.90
1:C:370:VAL:HG13	1:C:422:HIS:CD2	2.08	0.87
2:F:163:CYS:SG	2:F:174:CYS:CB	2.62	0.86
1:A:464:CYS:HG	1:A:524:CYS:HG	0.87	0.84
1:B:464:CYS:HG	1:B:524:CYS:HG	0.84	0.82
1:D:485:LEU:HD22	1:D:489:ARG:NH1	1.95	0.81
2:F:163:CYS:CB	2:F:174:CYS:SG	2.71	0.78
1:B:367:LYS:HG2	1:B:368:GLY:H	1.49	0.77
1:C:370:VAL:CG1	1:C:422:HIS:HD2	1.96	0.76
2:G:163:CYS:SG	2:G:174:CYS:CB	2.75	0.75
2:G:163:CYS:HB2	2:G:174:CYS:SG	2.28	0.73
2:H:259:CYS:HG	2:H:273:CYS:HG	1.32	0.71
2:H:181:THR:CG2	2:H:276:LYS:HE2	2.22	0.70
2:G:163:CYS:SG	2:G:164:PRO:HD2	2.35	0.66
1:D:358:CYS:HG	1:D:418:CYS:HG	0.68	0.66
2:G:176:TYR:HB3	2:G:282:CYS:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:223:LEU:HB3	2:E:260:VAL:HB	1.78	0.66
2:F:163:CYS:SG	2:F:164:PRO:HD2	2.36	0.66
2:G:172:ARG:NH1	2:G:285:LEU:CD2	2.60	0.65
2:G:163:CYS:CB	2:G:174:CYS:SG	2.85	0.64
1:B:367:LYS:HG2	1:B:368:GLY:N	2.12	0.64
1:C:366:SER:OG	1:C:367:LYS:N	2.30	0.64
2:E:223:LEU:HD11	2:E:232:PHE:HB3	1.81	0.63
2:G:172:ARG:HH12	2:G:285:LEU:CD2	2.13	0.62
2:E:163:CYS:HB3	2:E:174:CYS:SG	2.41	0.61
2:F:163:CYS:HG	2:F:174:CYS:HB3	1.64	0.61
2:G:172:ARG:HH12	2:G:285:LEU:HD21	1.66	0.59
1:D:360:VAL:HG13	1:D:399:VAL:HG13	1.85	0.59
1:B:360:VAL:HG13	1:B:399:VAL:HG13	1.86	0.58
1:C:360:VAL:HG13	1:C:399:VAL:HG13	1.86	0.58
1:A:360:VAL:HG13	1:A:399:VAL:HG13	1.86	0.57
1:C:370:VAL:HG23	1:C:387:ARG:HH22	1.69	0.56
2:H:181:THR:HG22	2:H:276:LYS:HE2	1.88	0.55
1:A:422:HIS:HB3	1:A:425:LEU:HB2	1.90	0.54
2:E:167:TRP:HB3	2:E:174:CYS:SG	2.48	0.53
1:C:439:PRO:HA	2:G:254:SER:HA	1.89	0.53
2:H:167:TRP:HB3	2:H:174:CYS:SG	2.49	0.53
2:H:176:TYR:HB3	2:H:282:CYS:HB2	1.93	0.51
2:G:172:ARG:NH2	2:G:285:LEU:HD22	2.25	0.51
1:B:514:ALA:O	1:B:518:GLN:HG3	2.10	0.51
1:B:363:LEU:HD22	3:J:1:NAG:H83	1.93	0.51
2:H:163:CYS:HB3	2:H:174:CYS:SG	2.52	0.50
1:C:363:LEU:HD22	3:K:1:NAG:H83	1.93	0.50
2:H:181:THR:HG22	2:H:276:LYS:CE	2.42	0.50
2:G:163:CYS:SG	2:G:164:PRO:CD	3.00	0.50
2:F:163:CYS:SG	2:F:164:PRO:CD	3.01	0.49
3:L:3:BMA:H61	3:L:5:MAN:H2	1.59	0.48
1:C:494:GLN:HE22	3:K:4:MAN:C3	2.27	0.48
2:F:184:TRP:HD1	2:F:220:TRP:CE3	2.31	0.48
2:G:184:TRP:HD1	2:G:220:TRP:CE3	2.31	0.48
2:E:184:TRP:HD1	2:E:220:TRP:CE3	2.31	0.48
2:H:184:TRP:HD1	2:H:220:TRP:CE3	2.31	0.47
1:B:373:THR:HB	1:B:419:ARG:HB3	1.96	0.47
2:E:191:CYS:HA	2:E:282:CYS:SG	2.54	0.47
1:A:373:THR:HB	1:A:419:ARG:HB3	1.96	0.47
1:B:452:GLU:OE2	1:B:457:ARG:CZ	2.63	0.46
1:B:452:GLU:HB2	1:B:460:ARG:NH2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:VAL:HB	1:C:403:LEU:HD11	1.99	0.45
1:B:382:VAL:HB	1:B:403:LEU:HD11	1.99	0.45
2:H:181:THR:HG21	2:H:276:LYS:HE2	1.96	0.45
1:D:382:VAL:HB	1:D:403:LEU:HD11	1.98	0.45
1:B:452:GLU:OE2	1:B:457:ARG:NE	2.50	0.44
1:A:382:VAL:HB	1:A:403:LEU:HD11	1.98	0.44
1:C:366:SER:OG	1:C:367:LYS:O	2.29	0.44
2:F:191:CYS:HA	2:F:282:CYS:SG	2.57	0.44
1:D:373:THR:HB	1:D:419:ARG:HB3	2.00	0.44
1:B:336:VAL:HG13	1:B:337:SER:N	2.31	0.43
2:H:226:LEU:HD23	2:H:228:LEU:HB3	2.01	0.43
1:B:439:PRO:HA	2:F:254:SER:HA	1.99	0.43
1:D:508:ARG:NH2	1:D:510:GLU:OE2	2.47	0.42
1:B:464:CYS:CB	1:B:524:CYS:HG	2.31	0.42
1:B:486:PRO:HD2	1:B:489:ARG:HG3	2.02	0.42
2:F:162:THR:HB	2:F:287:THR:HG23	2.02	0.42
2:G:162:THR:HB	2:G:287:THR:HG23	2.02	0.42
1:A:468:ASN:HA	1:A:502:GLY:HA3	2.01	0.41
1:D:485:LEU:HD22	1:D:489:ARG:HH11	1.80	0.41
1:C:486:PRO:HD2	1:C:489:ARG:HG3	2.01	0.41
1:D:531:ALA:HB1	1:D:537:VAL:HG23	2.03	0.41
1:A:531:ALA:HB1	1:A:537:VAL:HG23	2.03	0.41
2:E:163:CYS:SG	2:E:174:CYS:HB2	2.61	0.41
1:D:371:GLN:HB2	1:D:421:THR:HB	2.03	0.40
2:E:176:TYR:HB3	2:E:282:CYS:HB2	2.04	0.40
1:A:486:PRO:HD2	1:A:489:ARG:HG3	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:162:THR:CG2	2:H:276:LYS:NZ[1_666]	1.97	0.23

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	204/223 (92%)	194 (95%)	10 (5%)	0	100	100
1	B	209/223 (94%)	200 (96%)	8 (4%)	1 (0%)	24	59
1	C	209/223 (94%)	200 (96%)	8 (4%)	1 (0%)	24	59
1	D	204/223 (92%)	193 (95%)	10 (5%)	1 (0%)	24	59
2	E	128/143 (90%)	122 (95%)	6 (5%)	0	100	100
2	F	127/143 (89%)	119 (94%)	8 (6%)	0	100	100
2	G	129/143 (90%)	122 (95%)	7 (5%)	0	100	100
2	H	128/143 (90%)	121 (94%)	6 (5%)	1 (1%)	16	50
All	All	1338/1464 (91%)	1271 (95%)	63 (5%)	4 (0%)	36	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	368	GLY
1	B	371	GLN
1	C	371	GLN
2	H	291	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/195 (95%)	178 (96%)	7 (4%)	29	62
1	B	186/195 (95%)	176 (95%)	10 (5%)	20	53
1	C	186/195 (95%)	177 (95%)	9 (5%)	23	56
1	D	185/195 (95%)	177 (96%)	8 (4%)	26	59
2	E	114/120 (95%)	108 (95%)	6 (5%)	20	53
2	F	113/120 (94%)	106 (94%)	7 (6%)	16	49
2	G	114/120 (95%)	110 (96%)	4 (4%)	32	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	113/120 (94%)	110 (97%)	3 (3%)	39 68
All	All	1196/1260 (95%)	1142 (96%)	54 (4%)	24 58

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	360	VAL
1	A	370	VAL
1	A	378	SER
1	A	403	LEU
1	A	433	THR
1	A	475	SER
1	A	497	LYS
1	B	336	VAL
1	B	352	LYS
1	B	360	VAL
1	B	366	SER
1	B	371	GLN
1	B	403	LEU
1	B	425	LEU
1	B	427	ARG
1	B	433	THR
1	B	475	SER
1	C	360	VAL
1	C	367	LYS
1	C	369	THR
1	C	370	VAL
1	C	371	GLN
1	C	403	LEU
1	C	425	LEU
1	C	433	THR
1	C	475	SER
1	D	352	LYS
1	D	360	VAL
1	D	370	VAL
1	D	372	LEU
1	D	403	LEU
1	D	433	THR
1	D	475	SER
1	D	497	LYS
2	E	223	LEU
2	E	224	ARG

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Mol	Chain	Res	Type
2	E	228	LEU
2	E	252	SER
2	E	258	ASP
2	E	283	ASP
2	F	224	ARG
2	F	226	LEU
2	F	228	LEU
2	F	231	GLU
2	F	253	ARG
2	F	258	ASP
2	F	283	ASP
2	G	224	ARG
2	G	226	LEU
2	G	258	ASP
2	G	283	ASP
2	H	224	ARG
2	H	228	LEU
2	H	283	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	383	GLN
1	A	392	GLN
1	A	424	HIS
1	A	538	GLN
1	A	544	ASN
1	B	383	GLN
1	B	538	GLN
1	B	544	ASN
1	C	422	HIS
1	C	494	GLN
1	C	544	ASN
1	D	383	GLN
1	D	392	GLN
1	D	544	ASN
2	E	183	GLN
2	E	197	GLN
2	E	269	ASN
2	F	183	GLN
2	F	197	GLN
2	F	269	ASN

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Mol	Chain	Res	Type
2	G	255	GLN
2	G	269	ASN
2	H	197	GLN
2	H	255	GLN
2	H	269	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 ⓘ

20 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	1,3	14,14,15	0.25	0	17,19,21	0.78	1 (5%)
3	NAG	I	2	3	14,14,15	0.27	0	17,19,21	0.53	0
3	BMA	I	3	3	11,11,12	0.35	0	15,15,17	0.53	0
3	MAN	I	4	3	11,11,12	0.39	0	15,15,17	0.71	1 (6%)
3	MAN	I	5	3	11,11,12	0.38	0	15,15,17	1.17	1 (6%)
3	NAG	J	1	1,3	14,14,15	0.26	0	17,19,21	0.78	1 (5%)
3	NAG	J	2	3	14,14,15	0.28	0	17,19,21	0.54	0
3	BMA	J	3	3	11,11,12	0.30	0	15,15,17	0.49	0
3	MAN	J	4	3	11,11,12	0.34	0	15,15,17	0.79	1 (6%)
3	MAN	J	5	3	11,11,12	0.38	0	15,15,17	1.14	1 (6%)
3	NAG	K	1	1,3	14,14,15	0.28	0	17,19,21	0.80	1 (5%)
3	NAG	K	2	3	14,14,15	0.27	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	K	3	3	11,11,12	0.36	0	15,15,17	0.86	0
3	MAN	K	4	3	11,11,12	0.35	0	15,15,17	0.69	1 (6%)
3	MAN	K	5	3	11,11,12	0.43	0	15,15,17	1.00	1 (6%)
3	NAG	L	1	1,3	14,14,15	0.26	0	17,19,21	0.77	1 (5%)
3	NAG	L	2	3	14,14,15	0.29	0	17,19,21	0.54	0
3	BMA	L	3	3	11,11,12	0.29	0	15,15,17	0.89	1 (6%)
3	MAN	L	4	3	11,11,12	0.30	0	15,15,17	0.79	1 (6%)
3	MAN	L	5	3	11,11,12	0.41	0	15,15,17	0.94	1 (6%)

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	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	1/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
3	MAN	I	4	3	-	0/2/19/22	0/1/1/1
3	MAN	I	5	3	-	2/2/19/22	1/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	1/6/23/26	0/1/1/1
3	BMA	J	3	3	-	0/2/19/22	0/1/1/1
3	MAN	J	4	3	-	0/2/19/22	0/1/1/1
3	MAN	J	5	3	-	2/2/19/22	1/1/1/1
3	NAG	K	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	1/6/23/26	0/1/1/1
3	BMA	K	3	3	-	2/2/19/22	0/1/1/1
3	MAN	K	4	3	-	0/2/19/22	0/1/1/1
3	MAN	K	5	3	-	1/2/19/22	0/1/1/1
3	NAG	L	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	1/6/23/26	0/1/1/1
3	BMA	L	3	3	-	2/2/19/22	0/1/1/1
3	MAN	L	4	3	-	0/2/19/22	0/1/1/1
3	MAN	L	5	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	5	MAN	C1-O5-C5	4.31	117.97	112.19
3	J	5	MAN	C1-O5-C5	4.24	117.86	112.19
3	K	5	MAN	C1-O5-C5	3.24	116.52	112.19
3	L	5	MAN	C1-O5-C5	3.05	116.27	112.19
3	L	4	MAN	C1-O5-C5	2.59	115.66	112.19
3	J	4	MAN	C1-O5-C5	2.57	115.63	112.19
3	L	3	BMA	C1-O5-C5	2.54	115.59	112.19
3	K	1	NAG	O5-C1-C2	-2.31	107.72	111.29
3	I	1	NAG	O5-C1-C2	-2.29	107.74	111.29
3	J	1	NAG	O5-C1-C2	-2.28	107.76	111.29
3	L	1	NAG	O5-C1-C2	-2.28	107.77	111.29
3	I	4	MAN	C1-O5-C5	2.23	115.17	112.19
3	K	4	MAN	C1-O5-C5	2.21	115.14	112.19

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	3	BMA	O5-C5-C6-O6
3	J	5	MAN	C4-C5-C6-O6
3	K	3	BMA	C4-C5-C6-O6
3	J	5	MAN	O5-C5-C6-O6
3	I	5	MAN	C4-C5-C6-O6
3	I	5	MAN	O5-C5-C6-O6
3	L	3	BMA	O5-C5-C6-O6
3	L	3	BMA	C4-C5-C6-O6
3	K	5	MAN	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	5	MAN	C1-C2-C3-C4-C5-O5
3	I	5	MAN	C1-C2-C3-C4-C5-O5

5 monomers are involved in 4 short contacts:

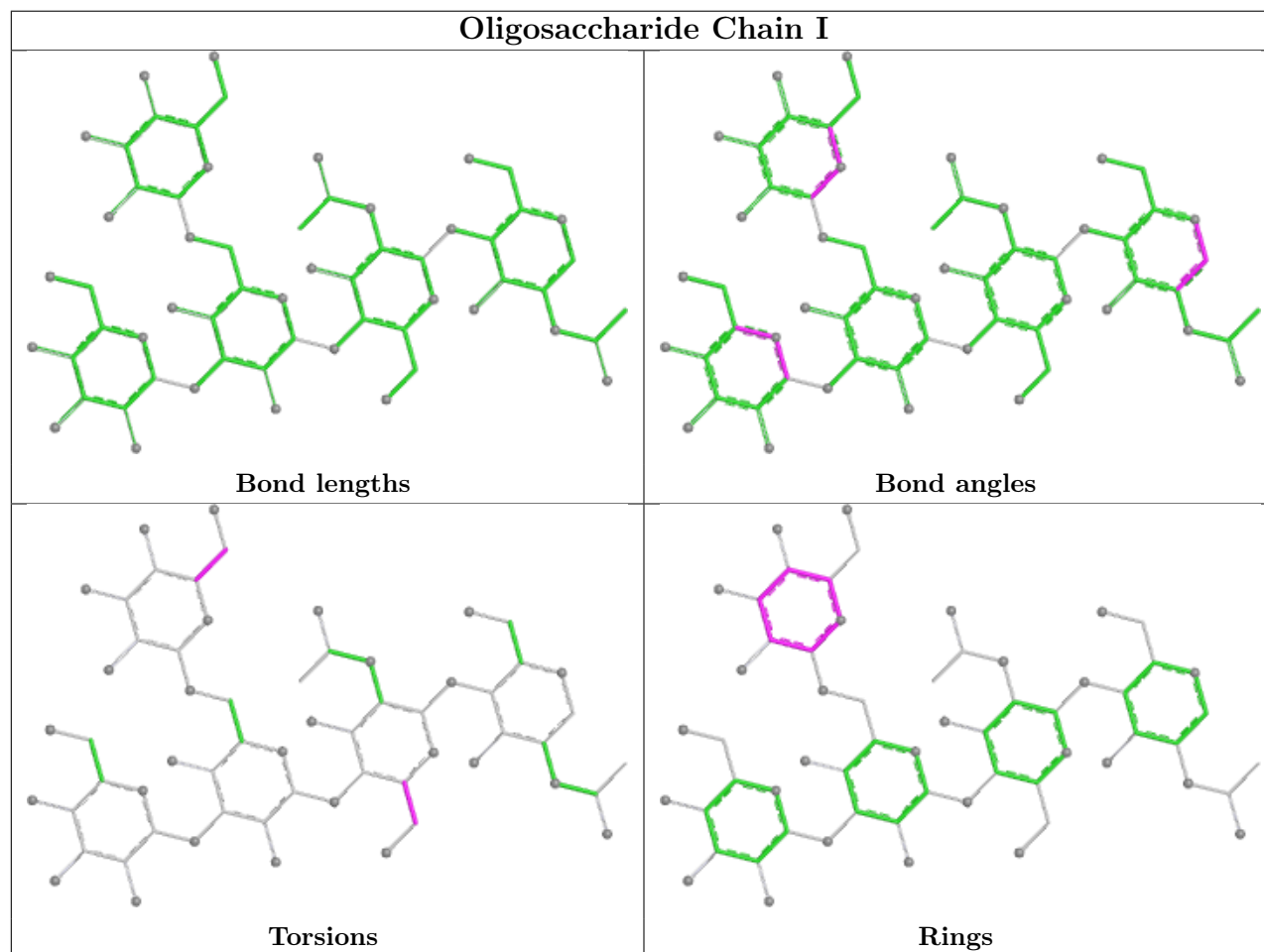
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	4	MAN	1	0

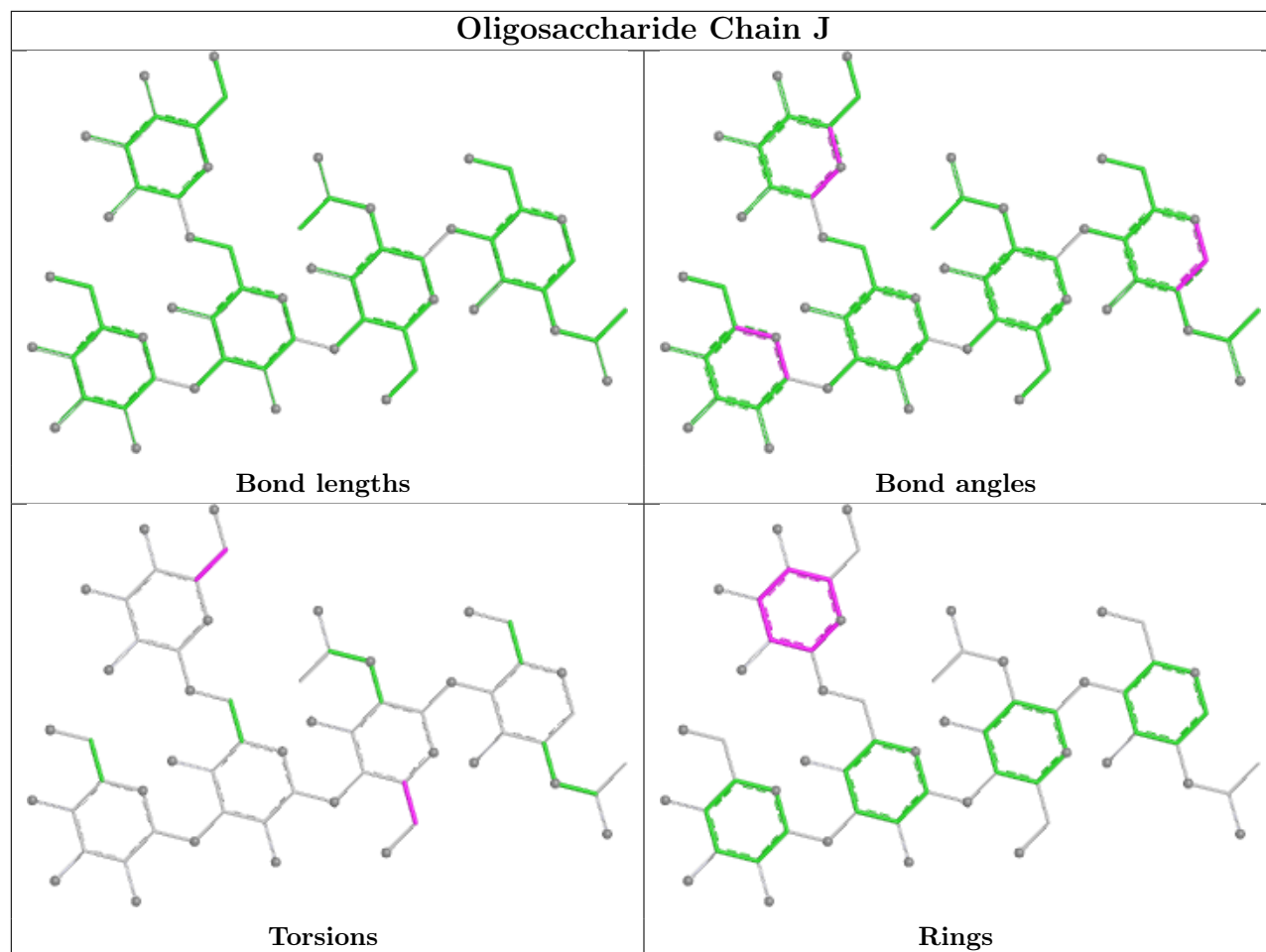
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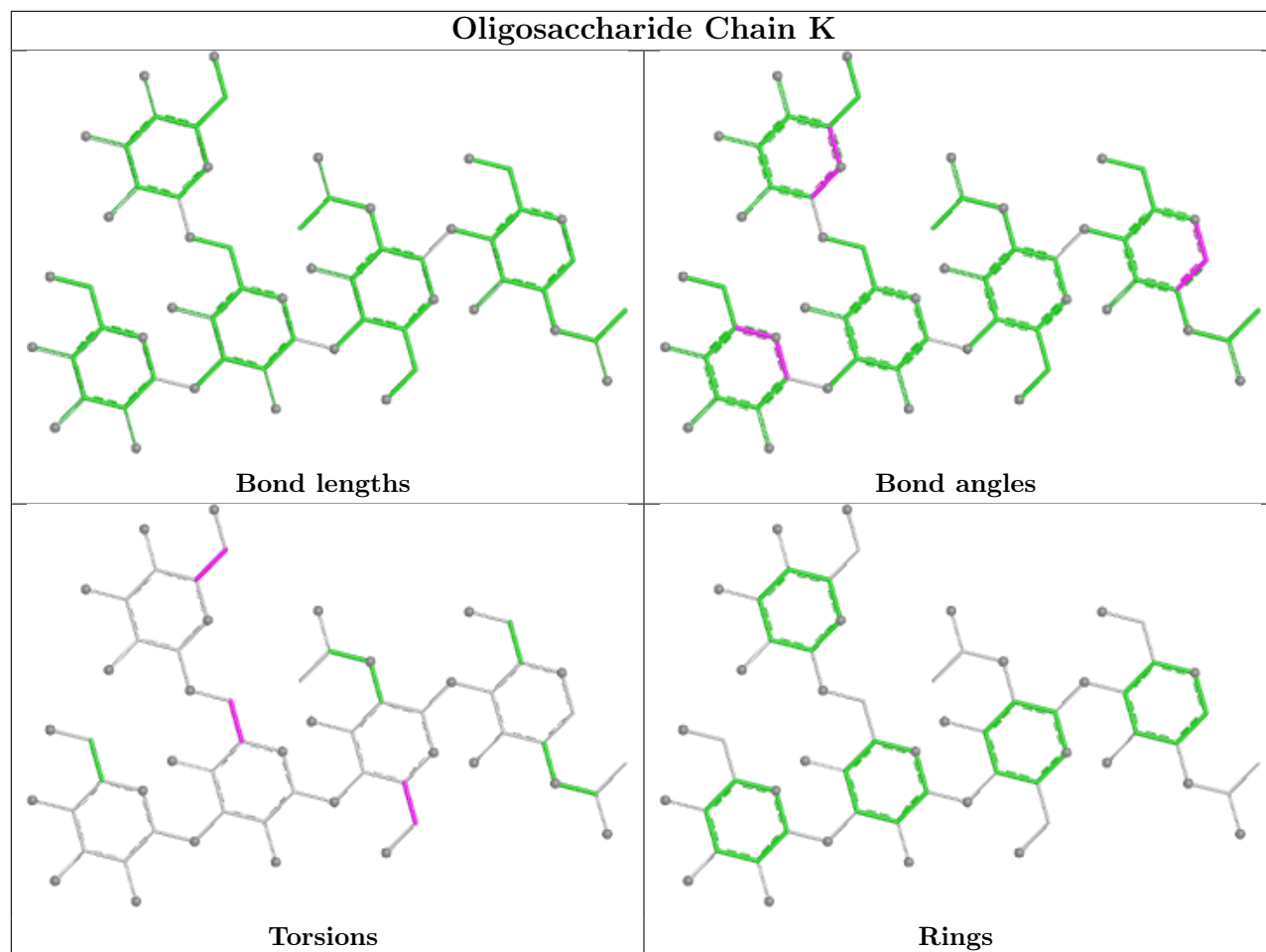
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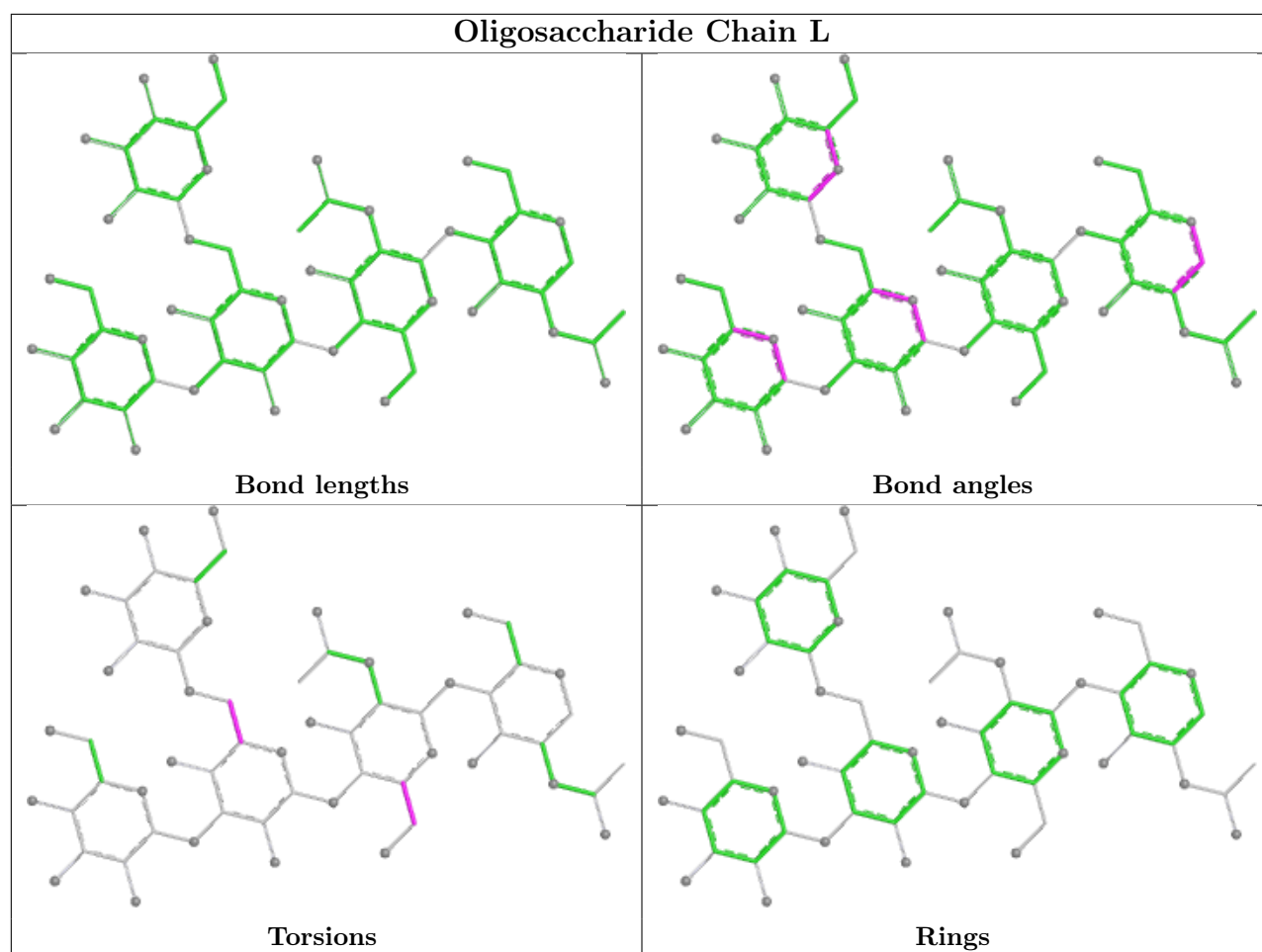
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	1	NAG	1	0
3	J	1	NAG	1	0
3	L	5	MAN	1	0
3	L	3	BMA	1	0

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](#)

There are no ligands in this entry.

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	208/223 (93%)	0.46	8 (3%)	44	27	40, 66, 105, 125	0
1	B	211/223 (94%)	0.57	10 (4%)	36	23	40, 67, 100, 112	0
1	C	211/223 (94%)	0.52	6 (2%)	55	35	40, 67, 95, 114	0
1	D	208/223 (93%)	0.55	5 (2%)	59	40	39, 64, 105, 131	0
2	E	132/143 (92%)	0.69	8 (6%)	27	17	58, 88, 115, 135	0
2	F	131/143 (91%)	1.10	19 (14%)	6	5	86, 103, 136, 169	0
2	G	133/143 (93%)	1.02	8 (6%)	27	17	47, 78, 97, 117	0
2	H	132/143 (92%)	0.88	9 (6%)	23	15	71, 102, 136, 148	0
All	All	1366/1464 (93%)	0.68	73 (5%)	32	20	39, 76, 118, 169	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	235	VAL	3.8
2	F	180	GLY	3.7
2	F	290	PRO	3.6
2	F	254	SER	3.6
1	D	362	ASP	3.5
2	H	292	ALA	3.5
2	F	229	LYS	3.5
2	H	180	GLY	3.5
2	F	289	THR	3.3
2	F	226	LEU	3.2
2	G	214	ALA	3.1
1	C	364	ALA	3.0
1	D	487	ASP	3.0
1	A	454	PRO	2.9
2	F	230	GLY	2.9
2	F	228	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	E	248	GLY	2.8
1	A	368	GLY	2.7
2	H	255	GLN	2.7
2	F	255	GLN	2.7
2	E	228	LEU	2.7
2	F	281	VAL	2.7
1	D	345	PRO	2.6
2	H	258	ASP	2.6
1	C	418	CYS	2.6
1	C	363	LEU	2.5
2	F	251	THR	2.5
2	F	239	HIS	2.5
1	A	535	GLN	2.5
2	G	180	GLY	2.5
2	F	201	ILE	2.4
2	F	258	ASP	2.4
1	C	368	GLY	2.4
1	B	418	CYS	2.4
2	F	162	THR	2.4
1	B	399	VAL	2.4
1	B	367	LYS	2.4
2	E	255	GLN	2.4
1	B	424	HIS	2.4
2	F	280	TRP	2.4
1	C	499	LYS	2.3
1	D	527	VAL	2.3
2	G	221	ILE	2.3
2	H	201	ILE	2.3
2	E	230	GLY	2.3
1	A	487	ASP	2.3
2	E	180	GLY	2.2
2	H	222	GLY	2.2
2	F	187	ALA	2.2
2	G	291	PRO	2.2
1	B	369	THR	2.2
1	A	382	VAL	2.2
2	G	226	LEU	2.2
1	D	365	PRO	2.2
1	B	529	GLU	2.2
1	A	362	ASP	2.1
1	B	337	SER	2.1
2	H	248	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	453	TRP	2.1
2	E	290	PRO	2.1
1	B	501	SER	2.1
2	G	177	PHE	2.1
2	H	254	SER	2.1
2	G	292	ALA	2.1
2	F	205	GLU	2.1
1	A	424	HIS	2.0
1	B	514	ALA	2.0
1	B	363	LEU	2.0
2	F	233	ILE	2.0
2	H	200	SER	2.0
1	A	476	VAL	2.0
2	E	226	LEU	2.0
2	E	221	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.

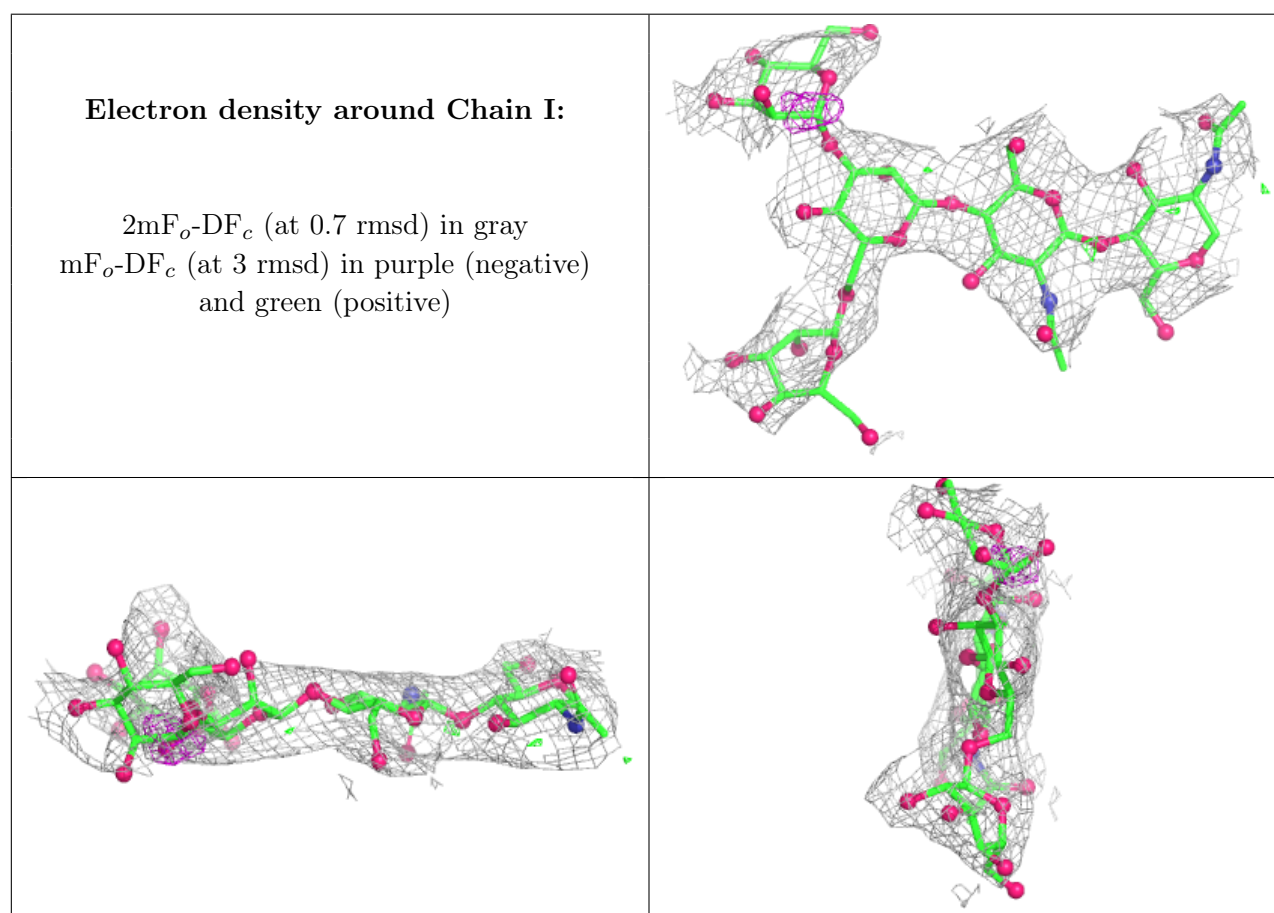
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	L	5	11/12	0.39	0.22	115,116,117,118	0
3	MAN	L	4	11/12	0.44	0.19	119,120,124,125	0
3	BMA	L	3	11/12	0.49	0.18	108,110,112,115	0
3	MAN	I	4	11/12	0.49	0.19	108,109,109,110	0
3	MAN	K	4	11/12	0.49	0.13	99,100,102,102	0
3	MAN	J	5	11/12	0.53	0.18	99,101,102,103	0
3	BMA	K	3	11/12	0.54	0.16	93,93,95,97	0
3	NAG	K	1	14/15	0.58	0.16	93,96,101,104	0
3	MAN	K	5	11/12	0.65	0.16	92,93,93,93	0
3	MAN	J	4	11/12	0.67	0.14	105,106,107,109	0
3	NAG	I	1	14/15	0.69	0.17	88,90,93,95	0
3	BMA	J	3	11/12	0.72	0.16	99,100,102,103	0
3	MAN	I	5	11/12	0.73	0.17	99,102,104,105	0

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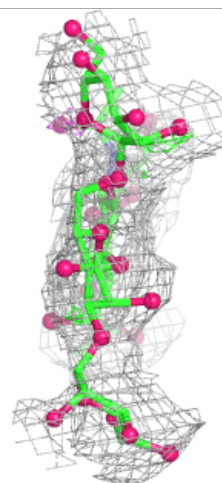
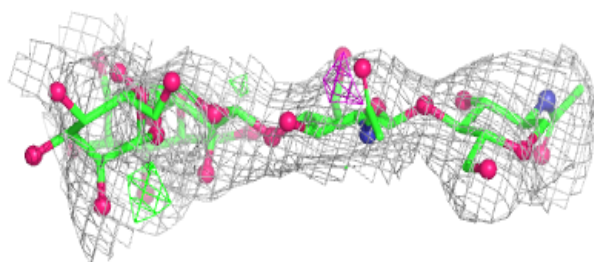
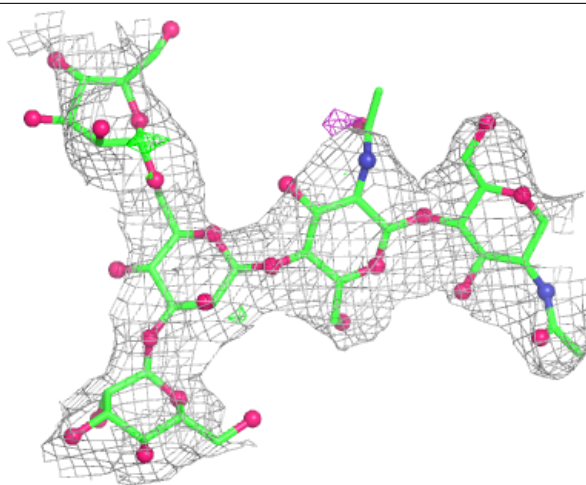
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	J	1	14/15	0.73	0.14	87,89,92,92	0
3	NAG	L	1	14/15	0.74	0.14	92,96,100,102	0
3	BMA	I	3	11/12	0.74	0.17	97,100,101,104	0
3	NAG	J	2	14/15	0.75	0.20	93,95,97,97	0
3	NAG	K	2	14/15	0.82	0.12	89,91,94,94	0
3	NAG	L	2	14/15	0.89	0.19	100,101,105,106	0
3	NAG	I	2	14/15	0.90	0.18	90,92,95,95	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.



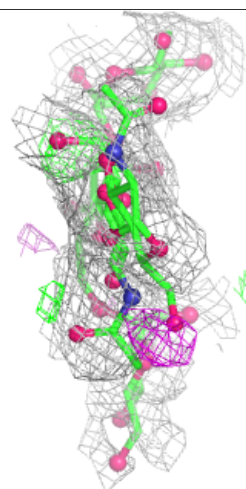
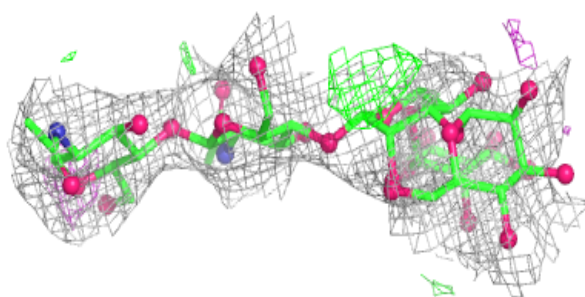
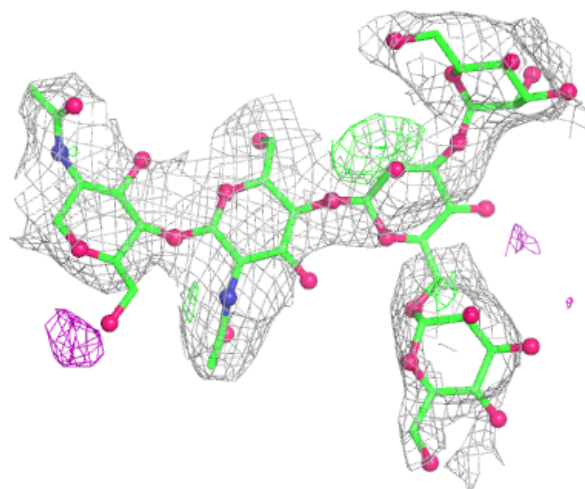
Electron density around Chain J:

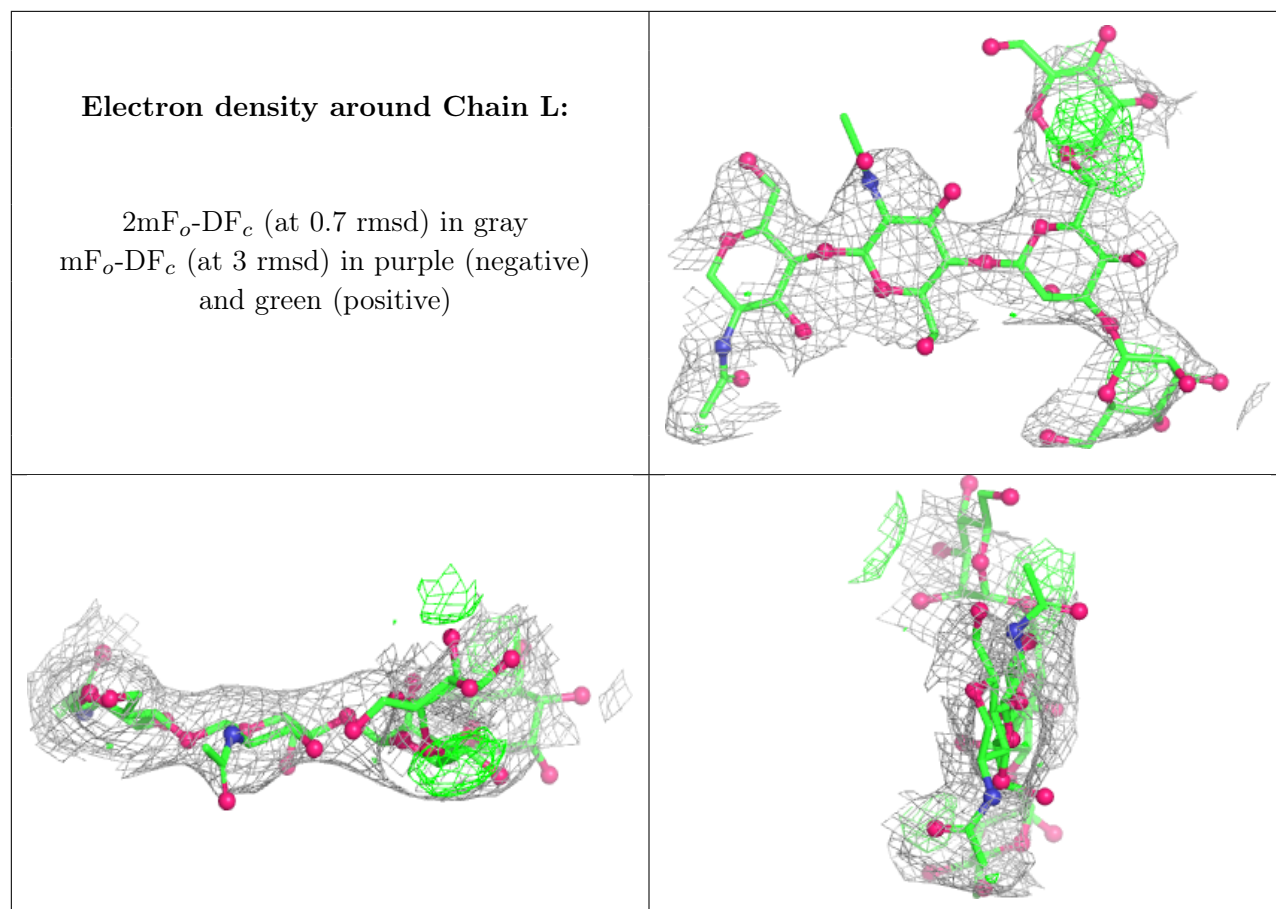
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.