



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:27 AM UTC

PDB ID : 2HIJ / pdb_00002hij
Title : Crystal Structure of P14 Alanine Variant of Antithrombin
Authors : Luis, S.A.; Bock, S.C.; Huntington, J.A.
Deposited on : 2006-06-29
Resolution : 2.90 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

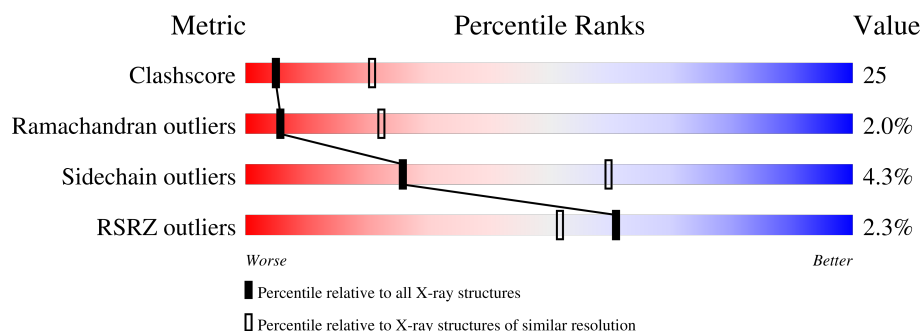
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	I	432	2% 53% 40% • 5%
2	L	432	2% 48% 43% • 5%
3	A	3	100%
4	B	2	50% 50%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6355 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 Antithrombin-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	411	Total	C	N	O	S	0	0	0
			3123	2009	514	584	16			

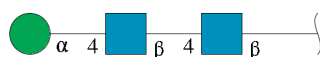
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	135	ALA	ASN	engineered mutation	UNP P01008
I	380	ALA	SER	engineered mutation	UNP P01008

- Molecule 2 is a protein called Antithrombin-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	409	Total	C	N	O	S	0	0	0
			3073	1972	507	577	17			

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



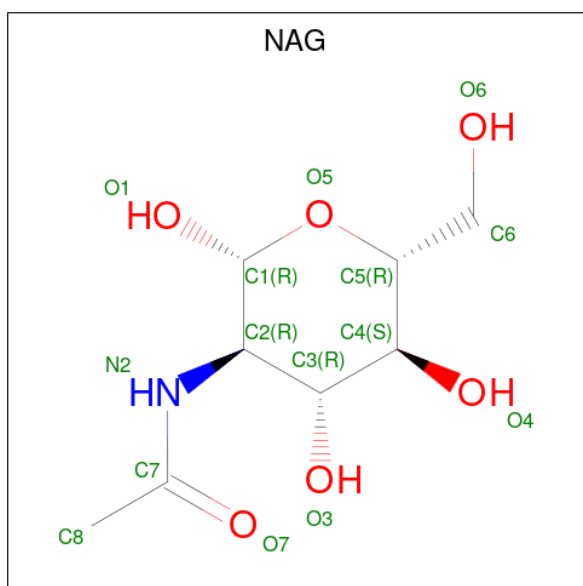
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	3	Total	C	N	O		0	0	0
			39	22	2	15				

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	I	1	Total	C	N	O	0	0
			14	8	1	5		
5	L	1	Total	C	N	O	0	0
			14	8	1	5		
5	L	1	Total	C	N	O	0	0
			14	8	1	5		
5	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	I	1	Total	C	O	0	0
			6	3	3		
6	L	1	Total	C	O	0	0
			6	3	3		

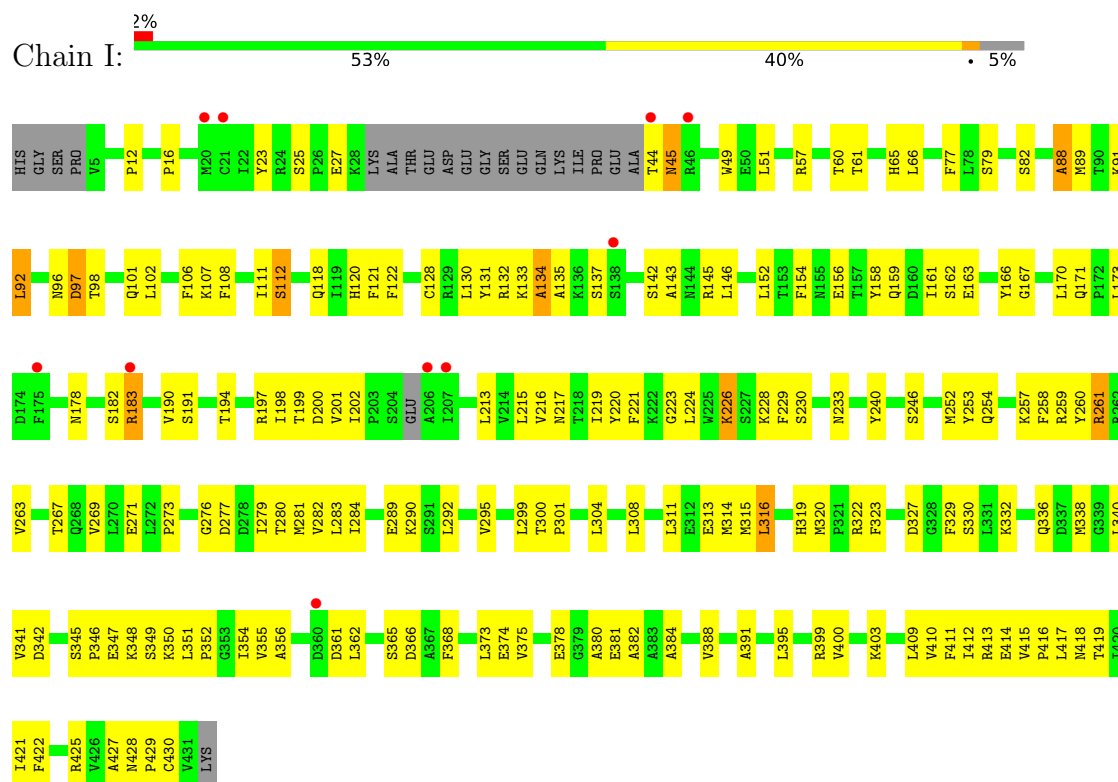
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	11	Total	O	0	0
			11	11		
7	L	13	Total	O	0	0
			13	13		

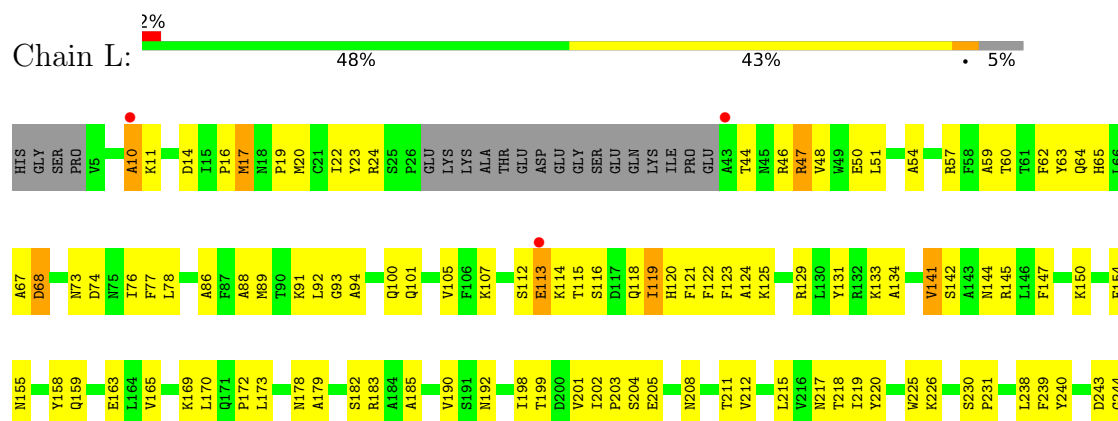
3 Residue-property plots

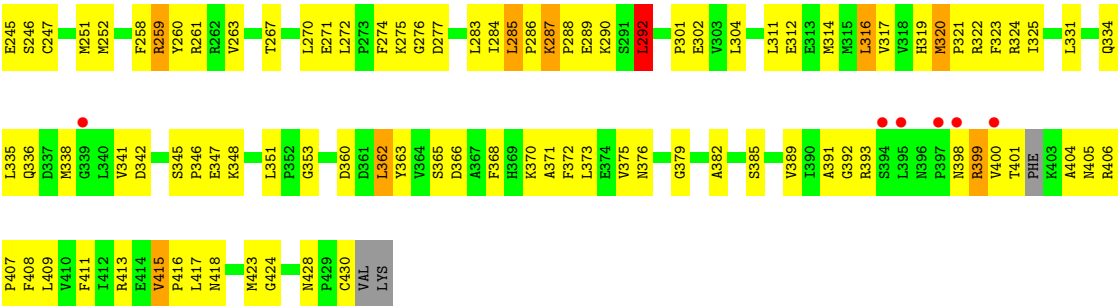
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Antithrombin-III

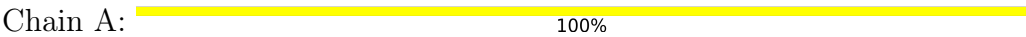


• Molecule 2: Antithrombin-III





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



● Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.74Å 98.63Å 87.57Å 90.00° 101.40° 90.00°	Depositor
Resolution (Å)	51.57 – 2.90 51.57 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (51.57-2.90) 99.3 (51.57-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.199 , 0.249 0.201 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	59.3	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 70.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6355	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.17% 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: GOL, MAN, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	I	0.48	0/3187	0.98	8/4332 (0.2%)
2	L	0.48	0/3136	0.97	10/4270 (0.2%)
All	All	0.48	0/6323	0.98	18/8602 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	382	ALA	N-CA-C	-9.89	94.81	110.14
2	L	226	LYS	N-CA-C	-6.76	103.94	111.71
1	I	88	ALA	N-CA-C	-6.72	104.03	111.36
2	L	415	VAL	N-CA-C	6.41	120.04	112.35
1	I	226	LYS	N-CA-C	-6.39	104.74	112.54
2	L	389	VAL	N-CA-C	6.19	116.78	107.80
1	I	228	LYS	N-CA-C	5.97	118.25	110.43
1	I	98	THR	N-CA-C	-5.96	104.47	110.97
1	I	329	PHE	N-CA-C	5.54	115.86	108.38
1	I	96	ASN	CB-CA-C	-5.43	110.29	116.54
2	L	341	VAL	N-CA-C	5.39	116.79	111.67
2	L	259	ARG	N-CA-C	-5.37	101.90	109.96
1	I	375	VAL	N-CA-C	5.23	115.59	107.28
2	L	292	LEU	N-CA-C	-5.17	105.64	111.28
2	L	287	LYS	CA-C-N	5.06	126.16	119.84
2	L	287	LYS	C-N-CA	5.06	126.16	119.84
2	L	362	LEU	N-CA-C	5.05	118.12	110.64
2	L	415	VAL	CB-CA-C	-5.04	107.40	114.00

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	I	3123	0	2968	144	0
2	L	3073	0	2878	163	0
3	A	39	0	34	3	0
4	B	28	0	25	0	0
5	I	14	0	13	0	0
5	L	42	0	39	4	0
6	I	6	0	8	1	0
6	L	6	0	8	0	0
7	I	11	0	0	1	0
7	L	13	0	0	0	0
All	All	6355	0	5973	308	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 25.

All (308) 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:I:213:LEU:HD11	1:I:354:ILE:HD13	1.34	1.09
2:L:86:ALA:HA	2:L:89:MET:HE3	1.51	0.92
2:L:192:ASN:HA	5:L:861:NAG:H62	1.53	0.91
1:I:350:LYS:HE2	3:A:1:NAG:H81	1.58	0.85
1:I:183:ARG:HB3	1:I:183:ARG:HH11	1.40	0.83
2:L:365:SER:HB3	2:L:392:GLY:H	1.42	0.82
2:L:159:GLN:HG3	2:L:170:LEU:HD12	1.61	0.82
1:I:223:GLY:H	1:I:380:ALA:HB3	1.46	0.80
2:L:62:PHE:HD1	2:L:338:MET:HE1	1.44	0.80
1:I:97:ASP:O	1:I:101:GLN:HG3	1.82	0.80
2:L:62:PHE:CD1	2:L:338:MET:HE1	2.17	0.78
2:L:23:TYR:HB3	2:L:116:SER:OG	1.83	0.78
1:I:258:PHE:HD2	1:I:316:LEU:HD21	1.49	0.77
1:I:146:LEU:HD13	1:I:215:LEU:HD13	1.65	0.77
1:I:319:HIS:HB2	1:I:403:LYS:HA	1.66	0.76
2:L:251:MET:HE3	2:L:319:HIS:HB3	1.68	0.75
2:L:91:LYS:HE2	2:L:120:HIS:NE2	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:124:ALA:HB2	2:L:165:VAL:HG13	1.69	0.73
1:I:281:MET:HE3	1:I:283:LEU:HD21	1.71	0.72
1:I:152:LEU:HD23	1:I:356:ALA:HB2	1.71	0.72
1:I:173:LEU:HD13	1:I:182:SER:HB3	1.71	0.72
1:I:292:LEU:HD11	1:I:409:LEU:HG	1.72	0.71
2:L:198:ILE:HG23	2:L:370:LYS:HG2	1.74	0.70
1:I:82:SER:HB2	1:I:219:ILE:HG13	1.73	0.70
2:L:208:ASN:HD22	2:L:393:ARG:HB2	1.57	0.68
2:L:239:PHE:O	2:L:246:SER:HB2	1.93	0.68
1:I:223:GLY:N	1:I:380:ALA:HB3	2.08	0.68
1:I:336:GLN:HA	1:I:340:LEU:O	1.94	0.68
1:I:143:ALA:O	1:I:217:ASN:HA	1.94	0.66
1:I:133:LYS:O	1:I:135:ALA:N	2.29	0.66
2:L:225:TRP:CD1	2:L:379:GLY:HA2	2.30	0.65
2:L:243:ASP:OD1	2:L:244:GLY:N	2.26	0.65
2:L:258:PHE:HB2	2:L:316:LEU:HD21	1.77	0.65
2:L:211:THR:HA	2:L:391:ALA:O	1.97	0.65
2:L:285:LEU:N	2:L:285:LEU:HD23	2.12	0.64
2:L:292:LEU:CD2	2:L:407:PRO:HG2	2.28	0.64
1:I:415:VAL:HB	1:I:416:PRO:HD3	1.80	0.64
1:I:351:LEU:HD23	1:I:354:ILE:HD12	1.80	0.64
2:L:144:ASN:HD22	2:L:217:ASN:HA	1.63	0.64
2:L:94:ALA:HA	2:L:351:LEU:HD23	1.80	0.64
1:I:92:LEU:HB3	1:I:158:TYR:CE1	2.33	0.64
1:I:183:ARG:HH11	1:I:183:ARG:CB	2.11	0.64
2:L:292:LEU:HD11	2:L:408:PHE:HA	1.80	0.63
1:I:152:LEU:CD2	1:I:356:ALA:HB2	2.27	0.63
2:L:47:ARG:HG2	2:L:122:PHE:CE2	2.34	0.63
2:L:47:ARG:HG2	2:L:122:PHE:CZ	2.34	0.63
2:L:292:LEU:HD21	2:L:407:PRO:O	1.99	0.63
1:I:154:PHE:HB3	1:I:170:LEU:HD13	1.79	0.63
1:I:259:ARG:HD3	1:I:271:GLU:OE1	2.00	0.62
2:L:91:LYS:CE	2:L:120:HIS:NE2	2.62	0.62
2:L:24:ARG:HA	2:L:114:LYS:O	1.99	0.62
1:I:213:LEU:CD1	1:I:354:ILE:HD13	2.20	0.62
1:I:281:MET:HE1	1:I:320:MET:HE1	1.82	0.61
3:A:1:NAG:H61	3:A:2:NAG:N2	2.16	0.60
1:I:315:MET:HE2	1:I:395:LEU:CD2	2.32	0.60
2:L:163:GLU:OE2	2:L:169:LYS:HG2	2.00	0.60
1:I:16:PRO:HD2	1:I:161:ILE:HD11	1.81	0.60
2:L:23:TYR:CE1	2:L:100:GLN:HG3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:63:TYR:HB2	2:L:423:MET:CE	2.31	0.60
1:I:130:LEU:CD2	1:I:414:GLU:HG3	2.32	0.60
2:L:51:LEU:HD21	2:L:123:PHE:HA	1.84	0.60
2:L:77:PHE:CE2	2:L:373:LEU:HB2	2.37	0.60
2:L:258:PHE:HB2	2:L:316:LEU:CD2	2.31	0.60
1:I:269:VAL:CG1	1:I:311:LEU:HD21	2.32	0.59
1:I:92:LEU:HB3	1:I:158:TYR:HE1	1.66	0.59
1:I:130:LEU:HD21	1:I:414:GLU:HG3	1.83	0.59
1:I:229:PHE:CE2	1:I:254:GLN:HG2	2.36	0.59
2:L:23:TYR:O	2:L:115:THR:HA	2.03	0.58
2:L:271:GLU:OE2	2:L:413:ARG:NH1	2.37	0.58
1:I:16:PRO:HG2	1:I:161:ILE:HD11	1.86	0.58
1:I:12:PRO:HG3	1:I:121:PHE:CZ	2.38	0.58
1:I:57:ARG:HG2	1:I:301:PRO:HG2	1.85	0.58
1:I:92:LEU:HD11	1:I:161:ILE:CG2	2.34	0.58
1:I:77:PHE:O	1:I:327:ASP:HB3	2.04	0.57
2:L:141:VAL:HG22	2:L:220:TYR:HB3	1.86	0.57
2:L:131:TYR:CE1	2:L:142:SER:HB2	2.40	0.57
2:L:201:VAL:HG11	2:L:385:SER:HB3	1.87	0.57
1:I:16:PRO:CG	1:I:161:ILE:HD11	2.35	0.56
1:I:213:LEU:HD11	1:I:354:ILE:CD1	2.23	0.56
2:L:347:GLU:OE1	2:L:347:GLU:N	2.28	0.56
2:L:323:PHE:HD2	2:L:325:ILE:HG23	1.71	0.56
2:L:91:LYS:NZ	2:L:120:HIS:NE2	2.53	0.56
2:L:287:LYS:O	2:L:289:GLU:N	2.38	0.56
1:I:45:ASN:N	1:I:45:ASN:HD22	2.02	0.56
1:I:323:PHE:HE2	1:I:373:LEU:HD23	1.69	0.56
5:L:801:NAG:H82	5:L:801:NAG:H3	1.88	0.56
2:L:46:ARG:O	2:L:50:GLU:HG3	2.05	0.56
1:I:154:PHE:CB	1:I:170:LEU:HD13	2.35	0.55
1:I:345:SER:HB3	1:I:348:LYS:HB2	1.88	0.55
2:L:322:ARG:O	2:L:322:ARG:HG2	2.07	0.55
2:L:346:PRO:HG3	2:L:363:TYR:CE2	2.42	0.55
1:I:92:LEU:HD11	1:I:161:ILE:HG22	1.88	0.55
1:I:263:VAL:HG22	1:I:267:THR:O	2.08	0.54
2:L:144:ASN:ND2	2:L:217:ASN:HA	2.22	0.54
1:I:154:PHE:CD2	1:I:170:LEU:HB3	2.42	0.54
1:I:412:ILE:HB	1:I:422:PHE:HB2	1.90	0.54
1:I:51:LEU:HD22	1:I:122:PHE:HB2	1.90	0.54
1:I:226:LYS:HE3	1:I:277:ASP:OD2	2.07	0.54
2:L:263:VAL:HG22	2:L:267:THR:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:190:VAL:HG21	1:I:201:VAL:HG21	1.89	0.54
1:I:354:ILE:HG22	1:I:362:LEU:HD13	1.90	0.54
2:L:73:ASN:HB3	2:L:404:ALA:N	2.23	0.54
2:L:73:ASN:HB3	2:L:404:ALA:H	1.73	0.54
1:I:425:ARG:HD3	1:I:427:ALA:HB2	1.90	0.53
2:L:360:ASP:C	2:L:362:LEU:H	2.16	0.53
2:L:398:ASN:O	2:L:399:ARG:C	2.50	0.53
2:L:251:MET:CE	2:L:319:HIS:HB3	2.37	0.53
2:L:260:TYR:CG	2:L:261:ARG:N	2.77	0.53
1:I:60:THR:HG21	1:I:300:THR:HA	1.89	0.53
1:I:313:GLU:O	1:I:314:MET:HB2	2.09	0.53
2:L:88:ALA:O	2:L:120:HIS:HE1	1.91	0.53
2:L:154:PHE:O	2:L:155:ASN:C	2.50	0.53
1:I:16:PRO:CD	1:I:161:ILE:HD11	2.38	0.53
1:I:191:SER:OG	1:I:199:THR:HG22	2.08	0.53
1:I:315:MET:HE2	1:I:395:LEU:HD21	1.90	0.53
1:I:91:LYS:NZ	1:I:120:HIS:NE2	2.37	0.53
1:I:314:MET:HE1	1:I:400:VAL:HG21	1.90	0.53
2:L:10:ALA:HB1	2:L:14:ASP:CB	2.39	0.53
2:L:334:GLN:CD	2:L:334:GLN:H	2.17	0.52
2:L:225:TRP:NE1	2:L:379:GLY:HA2	2.25	0.52
1:I:49:TRP:CZ3	1:I:417:LEU:HD22	2.45	0.52
1:I:289:GLU:H	1:I:289:GLU:CD	2.17	0.52
2:L:62:PHE:HA	2:L:338:MET:HE1	1.91	0.52
2:L:342:ASP:OD1	2:L:348:LYS:HB3	2.08	0.52
1:I:388:VAL:HG22	2:L:317:VAL:HB	1.92	0.52
2:L:22:ILE:CG2	2:L:115:THR:HB	2.40	0.52
2:L:178:ASN:O	2:L:179:ALA:C	2.53	0.52
2:L:183:ARG:NH1	2:L:202:ILE:O	2.43	0.52
1:I:230:SER:HB3	1:I:233:ASN:ND2	2.25	0.52
2:L:62:PHE:CZ	2:L:331:LEU:HD22	2.44	0.52
1:I:111:ILE:O	1:I:112:SER:C	2.53	0.51
1:I:391:ALA:O	2:L:321:PRO:HD3	2.09	0.51
1:I:220:TYR:CE1	1:I:381:GLU:OE2	2.64	0.51
1:I:137:SER:OG	1:I:224:LEU:HD12	2.09	0.51
1:I:154:PHE:CG	1:I:170:LEU:HD13	2.46	0.51
2:L:47:ARG:HA	2:L:50:GLU:OE1	2.11	0.51
2:L:57:ARG:HA	2:L:301:PRO:CG	2.41	0.51
2:L:284:ILE:HB	2:L:409:LEU:HB2	1.91	0.51
1:I:12:PRO:HG3	1:I:121:PHE:CE2	2.46	0.51
1:I:273:PRO:HA	1:I:280:THR:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:101:GLN:NE2	1:I:342:ASP:OD1	2.44	0.51
1:I:145:ARG:HD3	1:I:171:GLN:HB2	1.93	0.51
2:L:101:GLN:O	2:L:105:VAL:HG23	2.11	0.51
2:L:159:GLN:CG	2:L:170:LEU:HD12	2.38	0.51
2:L:11:LYS:H	2:L:14:ASP:CB	2.24	0.51
2:L:259:ARG:HD3	2:L:271:GLU:OE1	2.11	0.51
2:L:292:LEU:CD2	2:L:292:LEU:H	2.24	0.51
1:I:354:ILE:CG2	1:I:362:LEU:HD13	2.41	0.50
1:I:421:ILE:HG22	1:I:422:PHE:CD2	2.46	0.50
1:I:428:ASN:OD1	1:I:430:CYS:HB2	2.11	0.50
2:L:238:LEU:HD23	2:L:247:CYS:O	2.11	0.50
2:L:263:VAL:CG2	2:L:267:THR:HB	2.42	0.50
2:L:192:ASN:HA	5:L:861:NAG:C6	2.34	0.50
1:I:51:LEU:HD22	1:I:122:PHE:CB	2.42	0.50
2:L:208:ASN:ND2	2:L:393:ARG:HB2	2.27	0.50
1:I:201:VAL:HG23	1:I:202:ILE:HG12	1.94	0.50
1:I:260:TYR:CG	1:I:261:ARG:N	2.80	0.50
1:I:258:PHE:HD2	1:I:316:LEU:CD2	2.22	0.50
2:L:400:VAL:O	2:L:401:THR:C	2.54	0.50
1:I:226:LYS:NZ	7:I:872:HOH:O	2.46	0.49
1:I:395:LEU:HB2	1:I:399:ARG:NH1	2.26	0.49
1:I:27:GLU:CD	1:I:27:GLU:H	2.20	0.49
1:I:91:LYS:CB	1:I:102:LEU:HD13	2.43	0.49
1:I:258:PHE:CD2	1:I:316:LEU:HD21	2.38	0.49
2:L:258:PHE:CE1	2:L:272:LEU:HD22	2.47	0.49
1:I:79:SER:HB2	1:I:422:PHE:CE1	2.48	0.49
1:I:323:PHE:CE2	1:I:373:LEU:HD23	2.48	0.49
2:L:405:ASN:O	2:L:406:ARG:C	2.55	0.49
1:I:349:SER:OG	1:I:351:LEU:HD13	2.13	0.48
2:L:57:ARG:HA	2:L:301:PRO:HG2	1.95	0.48
2:L:286:PRO:HD3	2:L:292:LEU:HD13	1.94	0.48
1:I:269:VAL:HG12	1:I:311:LEU:HD21	1.95	0.48
1:I:341:VAL:HG23	1:I:342:ASP:H	1.79	0.48
2:L:74:ASP:OD1	2:L:401:THR:HG23	2.13	0.48
2:L:261:ARG:HB3	2:L:311:LEU:HD23	1.94	0.48
2:L:77:PHE:O	2:L:371:ALA:HB3	2.14	0.48
1:I:163:GLU:O	1:I:167:GLY:HA2	2.13	0.48
1:I:290:LYS:HE2	1:I:295:VAL:HG23	1.95	0.48
2:L:292:LEU:N	2:L:292:LEU:HD22	2.28	0.48
1:I:88:ALA:O	1:I:120:HIS:HE1	1.97	0.48
2:L:217:ASN:HD21	2:L:219:ILE:HG13	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:77:PHE:CE1	2:L:373:LEU:HD22	2.49	0.48
2:L:322:ARG:NH1	2:L:376:ASN:HB2	2.29	0.48
1:I:65:HIS:O	1:I:66:LEU:C	2.56	0.47
2:L:91:LYS:HE2	2:L:120:HIS:CE1	2.49	0.47
2:L:62:PHE:HA	2:L:338:MET:CE	2.44	0.47
2:L:63:TYR:HB2	2:L:423:MET:HE3	1.97	0.47
1:I:346:PRO:O	1:I:361:ASP:HB2	2.14	0.47
2:L:163:GLU:OE2	2:L:169:LYS:HE2	2.14	0.47
1:I:257:LYS:HA	1:I:314:MET:O	2.14	0.47
2:L:323:PHE:CD2	2:L:325:ILE:HG23	2.48	0.47
2:L:112:SER:O	2:L:113:GLU:C	2.58	0.47
2:L:155:ASN:ND2	5:L:841:NAG:C7	2.77	0.47
2:L:89:MET:O	2:L:92:LEU:HB2	2.14	0.46
2:L:215:LEU:HD12	2:L:215:LEU:H	1.81	0.46
2:L:304:LEU:HD11	2:L:411:PHE:CE2	2.50	0.46
2:L:51:LEU:CD2	2:L:123:PHE:HA	2.44	0.46
2:L:204:SER:O	2:L:205:GLU:HB2	2.16	0.46
2:L:372:PHE:O	2:L:382:ALA:HA	2.14	0.46
1:I:159:GLN:HG2	1:I:170:LEU:HD12	1.98	0.46
1:I:221:PHE:CE1	1:I:279:ILE:HG21	2.51	0.46
2:L:77:PHE:CZ	2:L:373:LEU:HB2	2.51	0.46
1:I:23:TYR:HE2	1:I:25:SER:HB3	1.81	0.46
1:I:44:THR:O	1:I:45:ASN:HB2	2.14	0.46
1:I:191:SER:CB	1:I:199:THR:HG22	2.45	0.46
1:I:381:GLU:HG3	1:I:381:GLU:O	2.16	0.46
1:I:146:LEU:HD13	1:I:215:LEU:CD1	2.41	0.45
1:I:276:GLY:O	1:I:277:ASP:HB2	2.16	0.45
1:I:299:LEU:O	1:I:300:THR:HG22	2.16	0.45
1:I:332:LYS:CE	1:I:365:SER:O	2.63	0.45
2:L:63:TYR:HB2	2:L:423:MET:HE1	1.97	0.45
2:L:258:PHE:HB3	2:L:270:LEU:HD11	1.98	0.45
2:L:119:ILE:HG22	2:L:120:HIS:N	2.30	0.45
2:L:292:LEU:HD23	2:L:407:PRO:HG2	1.99	0.45
2:L:372:PHE:CD1	2:L:372:PHE:C	2.94	0.45
2:L:292:LEU:H	2:L:292:LEU:HD22	1.81	0.45
1:I:283:LEU:CD2	1:I:410:VAL:HG22	2.47	0.45
2:L:428:ASN:OD1	2:L:430:CYS:HB2	2.17	0.45
1:I:374:GLU:HB3	1:I:381:GLU:HB3	1.99	0.45
2:L:118:GLN:O	2:L:119:ILE:C	2.60	0.45
2:L:125:LYS:O	2:L:129:ARG:HG2	2.17	0.45
2:L:201:VAL:HG11	2:L:385:SER:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:284:ILE:HB	1:I:409:LEU:HB2	1.99	0.45
2:L:76:ILE:O	2:L:424:GLY:HA3	2.17	0.45
2:L:208:ASN:OD1	2:L:208:ASN:C	2.60	0.45
2:L:238:LEU:HD22	2:L:246:SER:OG	2.17	0.45
2:L:190:VAL:HG13	2:L:218:THR:HG22	1.98	0.45
1:I:350:LYS:O	1:I:352:PRO:HD2	2.17	0.45
1:I:261:ARG:HB3	1:I:311:LEU:HD23	1.98	0.44
2:L:77:PHE:CD2	2:L:371:ALA:HB1	2.51	0.44
2:L:276:GLY:O	2:L:277:ASP:HB2	2.16	0.44
1:I:131:TYR:CE1	1:I:142:SER:HB3	2.51	0.44
1:I:332:LYS:NZ	1:I:365:SER:O	2.49	0.44
2:L:365:SER:HB3	2:L:392:GLY:N	2.22	0.44
1:I:332:LYS:HE2	1:I:365:SER:O	2.16	0.44
1:I:332:LYS:HE3	1:I:366:ASP:CG	2.42	0.44
1:I:45:ASN:N	1:I:45:ASN:ND2	2.65	0.44
2:L:158:TYR:HB2	2:L:353:GLY:O	2.18	0.44
1:I:417:LEU:O	1:I:418:ASN:C	2.60	0.44
2:L:283:LEU:HD11	2:L:320:MET:CE	2.47	0.44
3:A:2:NAG:H61	3:A:3:MAN:H2	2.00	0.44
2:L:124:ALA:HB2	2:L:165:VAL:CG1	2.42	0.44
2:L:44:THR:O	2:L:48:VAL:HG23	2.17	0.43
1:I:282:VAL:HB	1:I:411:PHE:HB2	2.00	0.43
1:I:330:SER:HB2	1:I:368:PHE:HE1	1.82	0.43
1:I:61:THR:O	1:I:65:HIS:HD2	2.01	0.43
2:L:65:HIS:CD2	2:L:338:MET:HE2	2.52	0.43
2:L:283:LEU:HD11	2:L:320:MET:HE3	1.99	0.43
2:L:252:MET:SD	2:L:322:ARG:HB2	2.58	0.43
1:I:252:MET:SD	1:I:322:ARG:HG2	2.58	0.43
2:L:17:MET:O	2:L:19:PRO:HD3	2.18	0.43
2:L:60:THR:O	2:L:64:GLN:HG3	2.18	0.43
2:L:212:VAL:HG21	2:L:362:LEU:CD2	2.48	0.43
2:L:54:ALA:HB1	2:L:107:LYS:O	2.19	0.43
1:I:315:MET:HE2	1:I:395:LEU:HD22	2.01	0.43
2:L:150:LYS:HG3	2:L:172:PRO:HB2	2.01	0.43
2:L:335:LEU:HD23	2:L:335:LEU:HA	1.83	0.43
2:L:16:PRO:O	2:L:17:MET:C	2.62	0.43
2:L:20:MET:CE	2:L:353:GLY:HA2	2.48	0.43
1:I:191:SER:HB2	1:I:199:THR:HG22	2.01	0.42
1:I:281:MET:CE	1:I:320:MET:HE1	2.48	0.42
2:L:68:ASP:OD1	2:L:68:ASP:C	2.61	0.42
2:L:93:GLY:O	2:L:351:LEU:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:182:SER:O	2:L:185:ALA:HB3	2.19	0.42
2:L:203:PRO:HG3	2:L:368:PHE:CE1	2.54	0.42
2:L:345:SER:HB3	2:L:348:LYS:HB2	2.01	0.42
1:I:308:LEU:HD13	1:I:413:ARG:CZ	2.48	0.42
2:L:286:PRO:HG3	2:L:292:LEU:HD22	2.02	0.42
2:L:78:LEU:N	2:L:78:LEU:HD23	2.35	0.42
1:I:194:THR:HG21	1:I:198:ILE:HD12	2.00	0.42
2:L:321:PRO:O	2:L:323:PHE:HD1	2.03	0.42
2:L:316:LEU:O	2:L:316:LEU:HD23	2.19	0.42
1:I:161:ILE:O	1:I:162:SER:C	2.61	0.42
2:L:145:ARG:HG2	2:L:147:PHE:CZ	2.54	0.42
2:L:225:TRP:HZ2	2:L:375:VAL:HG13	1.85	0.42
2:L:314:MET:HE3	2:L:314:MET:HB2	1.87	0.42
2:L:179:ALA:HB1	2:L:208:ASN:HA	2.02	0.42
2:L:145:ARG:HG2	2:L:147:PHE:CE1	2.55	0.41
1:I:183:ARG:HH11	1:I:183:ARG:CG	2.33	0.41
1:I:197:ARG:NH1	1:I:381:GLU:OE1	2.53	0.41
1:I:378:GLU:HG2	1:I:384:ALA:O	2.20	0.41
2:L:121:PHE:O	2:L:124:ALA:HB3	2.20	0.41
1:I:341:VAL:HG23	1:I:342:ASP:N	2.35	0.41
1:I:354:ILE:HB	1:I:362:LEU:HD13	2.01	0.41
2:L:173:LEU:HD13	2:L:182:SER:HB3	2.03	0.41
1:I:131:TYR:CZ	1:I:142:SER:HB3	2.56	0.41
2:L:292:LEU:CD2	2:L:292:LEU:N	2.84	0.41
1:I:330:SER:HB2	1:I:368:PHE:CE1	2.55	0.41
2:L:230:SER:HA	2:L:231:PRO:HD3	1.96	0.41
2:L:274:PHE:O	2:L:275:LYS:C	2.64	0.41
1:I:202:ILE:HD11	1:I:216:VAL:HG21	2.03	0.41
1:I:304:LEU:HD23	6:I:863:GOL:H11	2.03	0.41
1:I:380:ALA:O	1:I:381:GLU:C	2.64	0.41
2:L:63:TYR:O	2:L:67:ALA:CB	2.69	0.41
2:L:240:TYR:CE1	2:L:244:GLY:O	2.74	0.41
2:L:287:LYS:C	2:L:289:GLU:N	2.79	0.41
2:L:334:GLN:CD	2:L:334:GLN:N	2.78	0.41
2:L:415:VAL:N	2:L:416:PRO:HD2	2.35	0.41
1:I:240:TYR:CD1	1:I:246:SER:HB3	2.56	0.40
1:I:336:GLN:C	1:I:338:MET:N	2.77	0.40
1:I:253:TYR:CD2	1:I:253:TYR:C	2.97	0.40
2:L:22:ILE:HG23	2:L:115:THR:HB	2.03	0.40
1:I:133:LYS:O	1:I:134:ALA:C	2.64	0.40
1:I:166:TYR:O	1:I:167:GLY:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:417:LEU:O	2:L:418:ASN:C	2.65	0.40
1:I:102:LEU:HD23	1:I:340:LEU:HD11	2.04	0.40
1:I:106:PHE:O	1:I:108:PHE:N	2.55	0.40
2:L:59:ALA:O	2:L:423:MET:HE1	2.21	0.40

There are no symmetry-related clashes.

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	I	405/432 (94%)	354 (87%)	44 (11%)	7 (2%)	7	26
2	L	403/432 (93%)	353 (88%)	41 (10%)	9 (2%)	5	20
All	All	808/864 (94%)	707 (88%)	85 (10%)	16 (2%)	6	22

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	107	LYS
1	I	112	SER
1	I	134	ALA
2	L	113	GLU
2	L	133	LYS
2	L	290	LYS
1	I	200	ASP
2	L	10	ALA
2	L	134	ALA
2	L	288	PRO
2	L	399	ARG
1	I	45	ASN
1	I	178	ASN
1	I	261	ARG

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Mol	Chain	Res	Type
2	L	17	MET
2	L	119	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	316/381 (83%)	303 (96%)	13 (4%)	27	61
2	L	306/383 (80%)	292 (95%)	14 (5%)	24	57
All	All	622/764 (81%)	595 (96%)	27 (4%)	26	60

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	89	MET
1	I	92	LEU
1	I	97	ASP
1	I	118	GLN
1	I	128	CYS
1	I	132	ARG
1	I	156	GLU
1	I	183	ARG
1	I	316	LEU
1	I	347	GLU
1	I	355	VAL
1	I	419	THR
1	I	429	PRO
2	L	47	ARG
2	L	68	ASP
2	L	141	VAL
2	L	199	THR
2	L	245	GLU
2	L	285	LEU
2	L	292	LEU
2	L	302	GLU

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Mol	Chain	Res	Type
2	L	312	GLU
2	L	316	LEU
2	L	320	MET
2	L	324	ARG
2	L	336	GLN
2	L	366	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	45	ASN
1	I	118	GLN
1	I	233	ASN
1	I	319	HIS
1	I	334	GLN
1	I	418	ASN
2	L	65	HIS
2	L	144	ASN
2	L	217	ASN
2	L	233	ASN
2	L	254	GLN
2	L	336	GLN
2	L	396	ASN
2	L	428	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 ⓘ

5 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	A	1	3,1	14,14,15	0.64	0	17,19,21	0.84	0
3	NAG	A	2	3	14,14,15	0.61	0	17,19,21	0.66	0
3	MAN	A	3	3	11,11,12	0.57	0	15,15,17	0.46	0
4	NAG	B	1	4,1	14,14,15	0.66	0	17,19,21	0.76	0
4	NAG	B	2	4	14,14,15	0.58	0	17,19,21	0.69	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
3	NAG	A	1	3,1	-	5/6/23/26	0/1/1/1
3	NAG	A	2	3	-	5/6/23/26	0/1/1/1
3	MAN	A	3	3	-	2/2/19/22	0/1/1/1
4	NAG	B	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	B	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2	NAG	C2-N2-C7	-2.06	120.14	122.90

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	NAG	C1-C2-N2-C7
3	A	1	NAG	C8-C7-N2-C2
3	A	1	NAG	O7-C7-N2-C2
3	A	2	NAG	C3-C2-N2-C7
3	A	2	NAG	C8-C7-N2-C2
3	A	2	NAG	O7-C7-N2-C2
4	B	1	NAG	C3-C2-N2-C7

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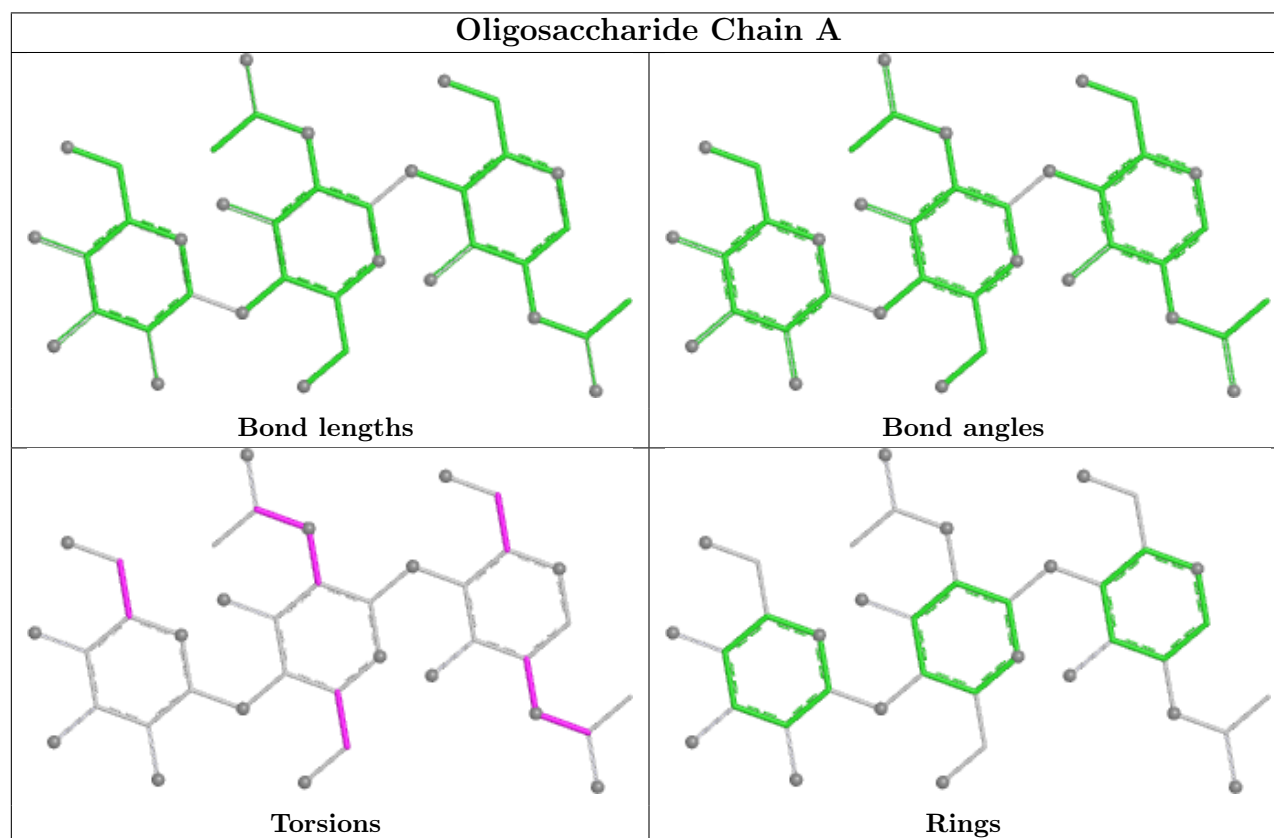
Mol	Chain	Res	Type	Atoms
4	B	1	NAG	C8-C7-N2-C2
4	B	1	NAG	O7-C7-N2-C2
4	B	2	NAG	C8-C7-N2-C2
4	B	2	NAG	O7-C7-N2-C2
3	A	1	NAG	O5-C5-C6-O6
3	A	2	NAG	O5-C5-C6-O6
3	A	3	MAN	O5-C5-C6-O6
3	A	3	MAN	C4-C5-C6-O6
3	A	1	NAG	C4-C5-C6-O6
3	A	2	NAG	C4-C5-C6-O6

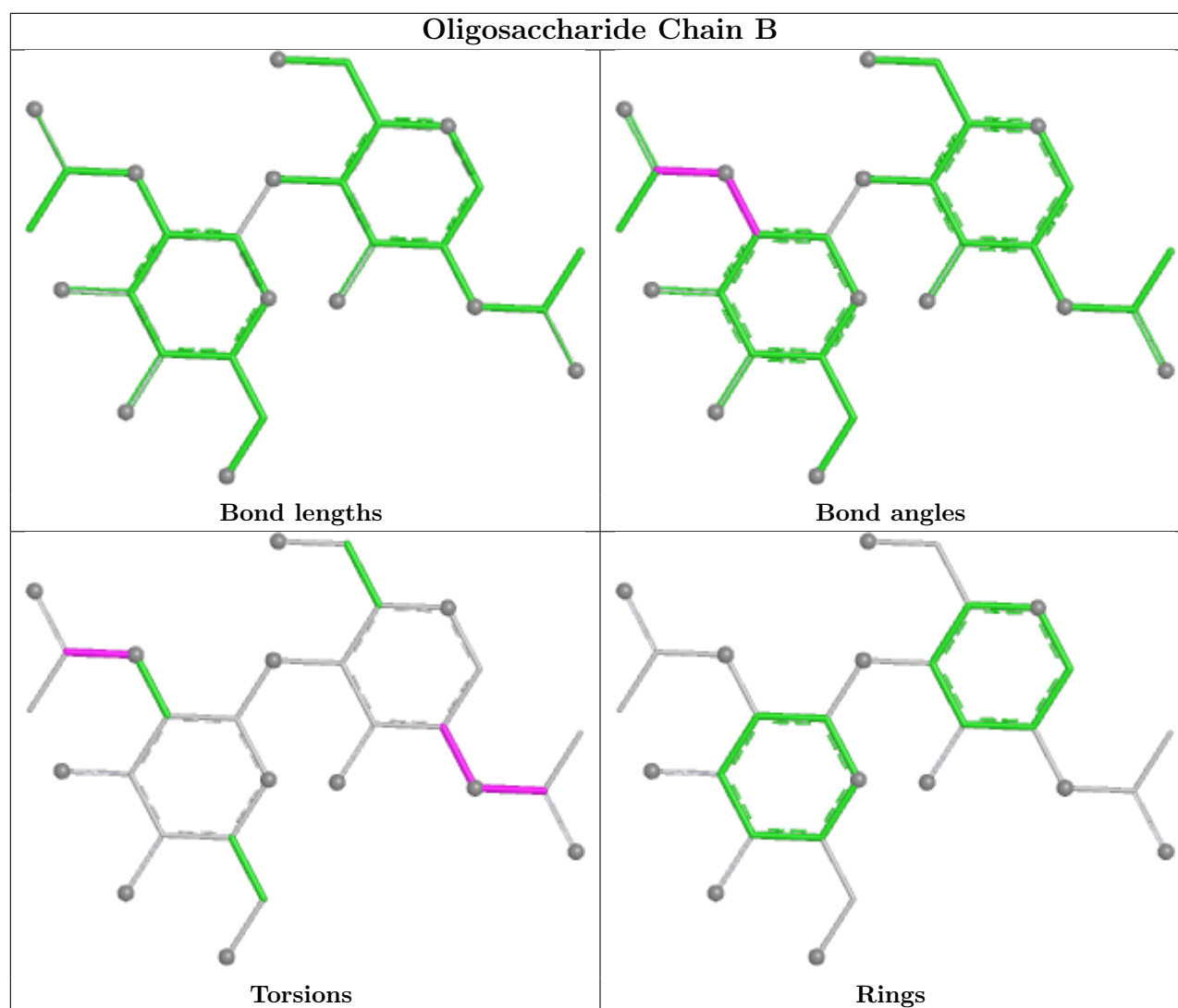
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2	NAG	2	0
3	A	1	NAG	2	0
3	A	3	MAN	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](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	L	841	2	14,14,15	0.69	0	17,19,21	0.81	1 (5%)
6	GOL	L	862	-	5,5,5	0.57	0	5,5,5	0.42	0
5	NAG	I	841	1	14,14,15	0.58	0	17,19,21	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	L	801	2	14,14,15	0.72	0	17,19,21	0.78	0
5	NAG	L	861	2	14,14,15	0.97	1 (7%)	17,19,21	1.37	3 (17%)
6	GOL	I	863	-	5,5,5	0.84	0	5,5,5	0.48	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	L	841	2	-	3/6/23/26	0/1/1/1
6	GOL	L	862	-	-	2/4/4/4	-
5	NAG	I	841	1	-	2/6/23/26	0/1/1/1
5	NAG	L	801	2	-	5/6/23/26	0/1/1/1
5	NAG	L	861	2	-	5/6/23/26	0/1/1/1
6	GOL	I	863	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	861	NAG	C1-C2	2.75	1.56	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	861	NAG	C1-O5-C5	3.60	117.01	112.19
5	L	861	NAG	O5-C1-C2	2.57	115.26	111.29
5	L	841	NAG	C4-C3-C2	2.37	114.48	111.02
5	L	861	NAG	C4-C3-C2	-2.16	107.86	111.02

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	841	NAG	C8-C7-N2-C2
5	I	841	NAG	O7-C7-N2-C2
5	L	801	NAG	C1-C2-N2-C7
5	L	801	NAG	C8-C7-N2-C2
5	L	801	NAG	O7-C7-N2-C2
5	L	841	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
5	L	841	NAG	C8-C7-N2-C2
5	L	841	NAG	O7-C7-N2-C2
5	L	861	NAG	C8-C7-N2-C2
5	L	861	NAG	O7-C7-N2-C2
6	L	862	GOL	O2-C2-C3-O3
5	L	861	NAG	O5-C5-C6-O6
5	L	801	NAG	O5-C5-C6-O6
5	L	801	NAG	C4-C5-C6-O6
6	L	862	GOL	C1-C2-C3-O3
5	L	861	NAG	C4-C5-C6-O6
5	L	861	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	841	NAG	1	0
5	L	801	NAG	1	0
5	L	861	NAG	2	0
6	I	863	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	I	411/432 (95%)	0.13	10 (2%) 59 50	20, 50, 83, 102	0
2	L	409/432 (94%)	0.10	9 (2%) 62 53	25, 49, 86, 112	0
All	All	820/864 (94%)	0.12	19 (2%) 61 52	20, 50, 84, 112	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	398	ASN	4.1
1	I	360	ASP	3.8
1	I	21	CYS	2.7
1	I	20	MET	2.7
1	I	207	ILE	2.6
2	L	397	PRO	2.4
1	I	175	PHE	2.4
2	L	394	SER	2.4
2	L	10	ALA	2.4
2	L	400	VAL	2.4
1	I	138	SER	2.3
2	L	395	LEU	2.3
2	L	43	ALA	2.3
2	L	113	GLU	2.2
1	I	46	ARG	2.2
1	I	44	THR	2.1
1	I	206	ALA	2.1
1	I	183	ARG	2.0
2	L	339	GLY	2.0

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

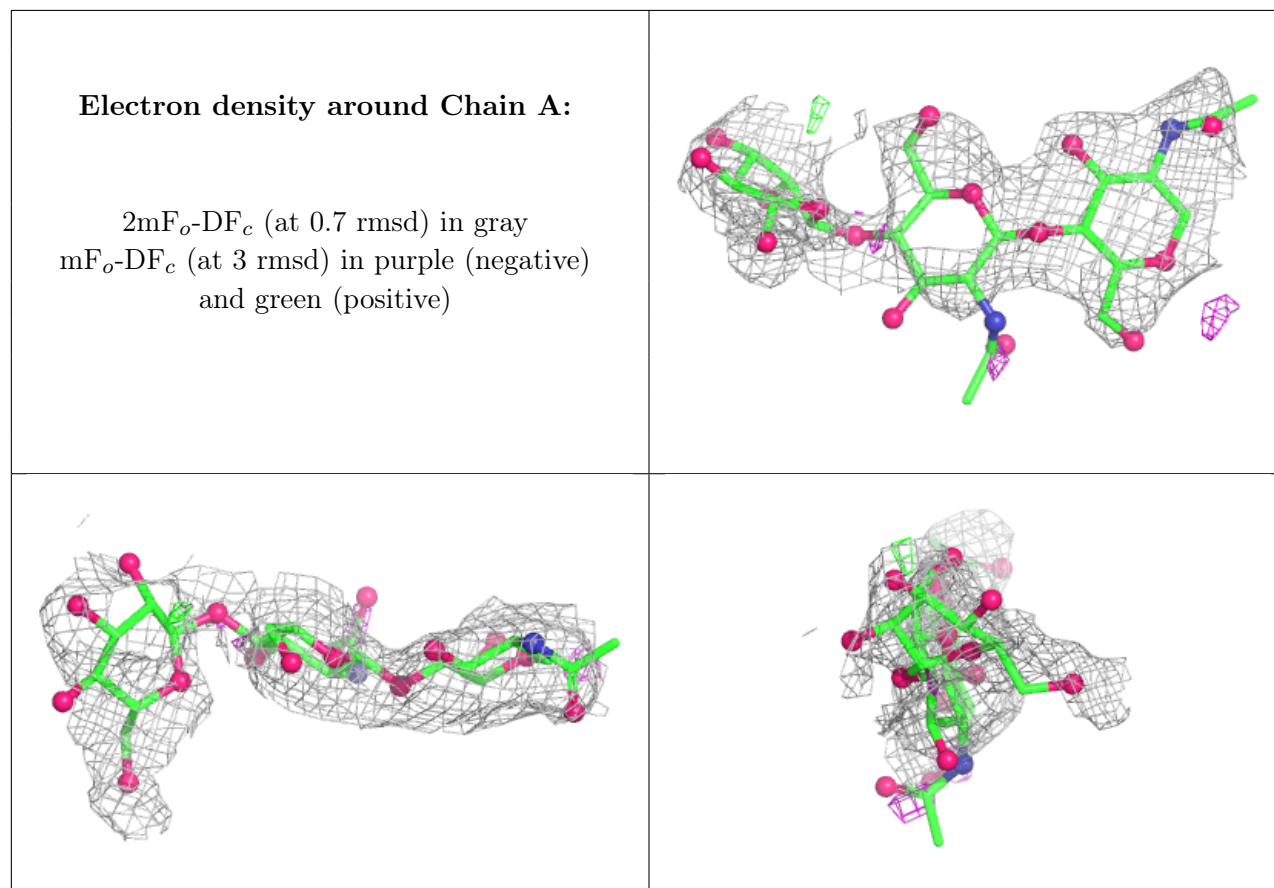
There are no non-standard protein/DNA/RNA residues in this entry.

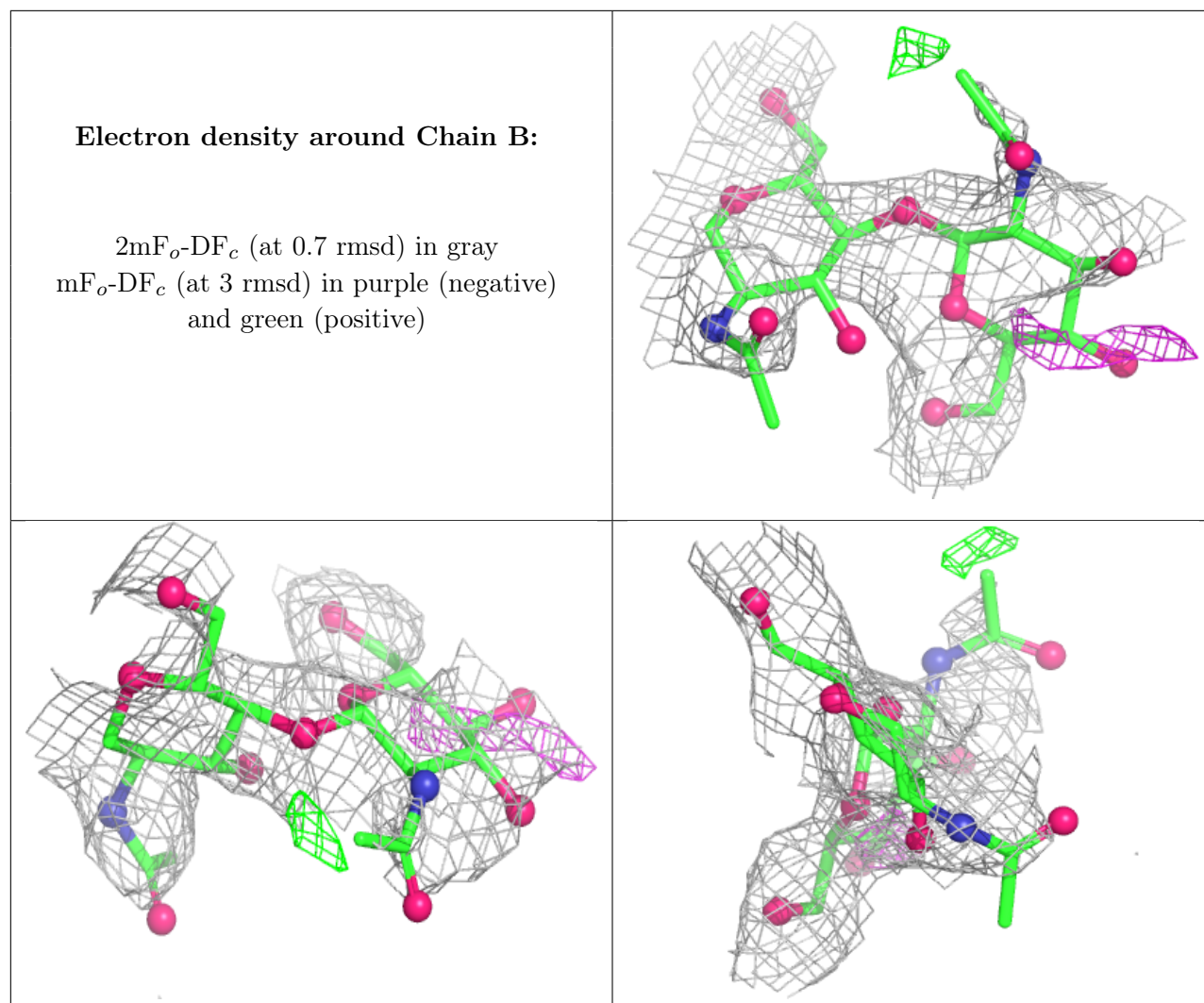
6.3 Carbohydrates [i](#)

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	NAG	A	1	14/15	-	-	100,106,111,119	0
3	NAG	A	2	14/15	-	-	126,131,134,135	0
3	MAN	A	3	11/12	-	-	134,135,135,136	0
4	NAG	B	1	14/15	-	-	118,124,127,131	0
4	NAG	B	2	14/15	-	-	136,138,139,140	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 ⓘ

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($\text{\AA}^2$)	Q<0.9
5	NAG	L	801	14/15	0.60	0.14	89,92,94,95	0
5	NAG	L	861	14/15	0.67	0.16	80,84,86,88	0
5	NAG	I	841	14/15	0.80	0.16	72,75,77,78	0
5	NAG	L	841	14/15	0.82	0.14	61,69,72,73	0
6	GOL	L	862	6/6	0.90	0.17	75,75,76,76	0
6	GOL	I	863	6/6	0.91	0.15	76,78,79,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.