



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 22, 2026 – 12:27 PM EDT

PDB ID : 9ZCJ / pdb_00009zsj
Title : Therapeutic antibody with captured antigen
Authors : Gorman, M.A.; Parker, M.W.
Deposited on : 2025-11-23
Resolution : 2.60 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

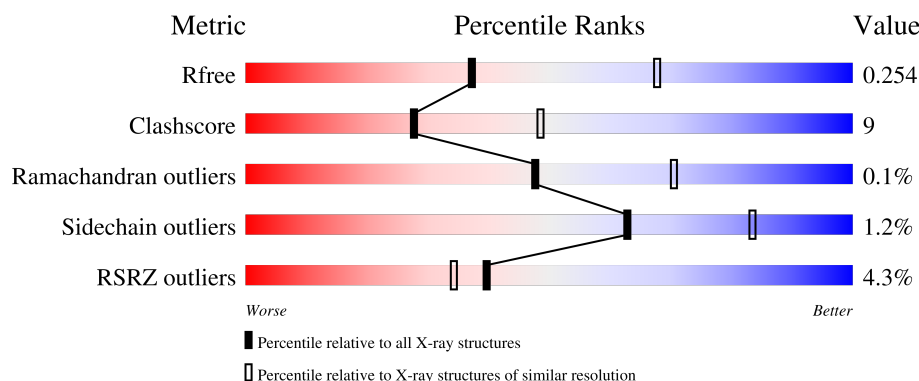
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	517	8% 71% 24% 5%
1	B	517	6% 72% 19% 9%
2	C	216	% 90% 9% .
2	G	216	% 92% 7% .
3	D	231	2% 89% 9% .

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Mol	Chain	Length	Quality of chain
3	I	231	% 87% 10% . .
4	E	3	100%
4	H	3	33% 67%
5	F	2	50% 50%
5	J	2	50% 50%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 28743 atoms, of which 14182 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 Serine protease complement C2b.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	492	Total	C	H	N	O	S	0	0	0
			7741	2445	3857	686	726	27			
1	B	473	Total	C	H	N	O	S	0	0	0
			7482	2368	3731	661	695	27			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	733	HIS	-	expression tag	UNP P06681
A	734	HIS	-	expression tag	UNP P06681
A	735	HIS	-	expression tag	UNP P06681
A	736	HIS	-	expression tag	UNP P06681
A	737	HIS	-	expression tag	UNP P06681
A	738	HIS	-	expression tag	UNP P06681
A	739	HIS	-	expression tag	UNP P06681
A	740	HIS	-	expression tag	UNP P06681
B	733	HIS	-	expression tag	UNP P06681
B	734	HIS	-	expression tag	UNP P06681
B	735	HIS	-	expression tag	UNP P06681
B	736	HIS	-	expression tag	UNP P06681
B	737	HIS	-	expression tag	UNP P06681
B	738	HIS	-	expression tag	UNP P06681
B	739	HIS	-	expression tag	UNP P06681
B	740	HIS	-	expression tag	UNP P06681

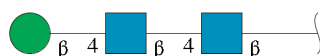
- Molecule 2 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	214	Total	C	H	N	O	S	0	0	0
			3139	992	1548	270	324	5			
2	G	215	Total	C	H	N	O	S	0	0	0
			3159	997	1559	272	326	5			

- Molecule 3 is a protein called Fab heavy chain.

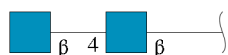
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	225	Total	C	H	N	O	S	0	0	0
			3359	1082	1654	278	336	9			
3	I	225	Total	C	H	N	O	S	0	1	0
			3359	1082	1654	278	336	9			

- Molecule 4 is an oligosaccharide called 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
4	E	3	Total	C	H	N	O		0	0	0
			73	22	34	2	15				
4	H	3	Total	C	H	N	O		0	0	0
			73	22	34	2	15				

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

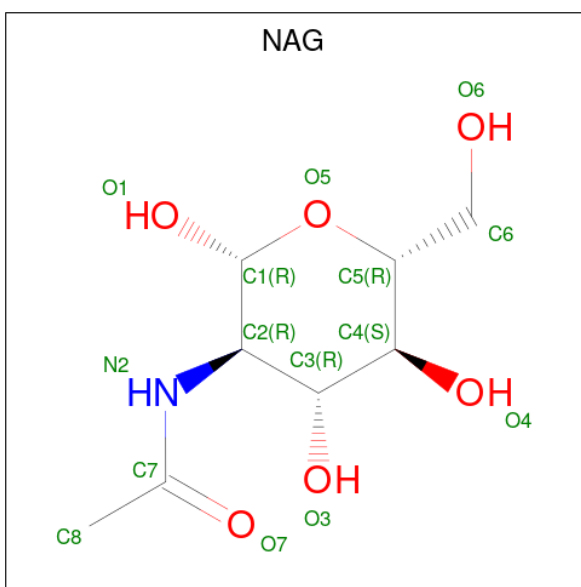


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	F	2	Total	C	H	N	O		0	0	0
			53	16	25	2	10				
5	J	2	Total	C	H	N	O		0	0	0
			53	16	25	2	10				

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

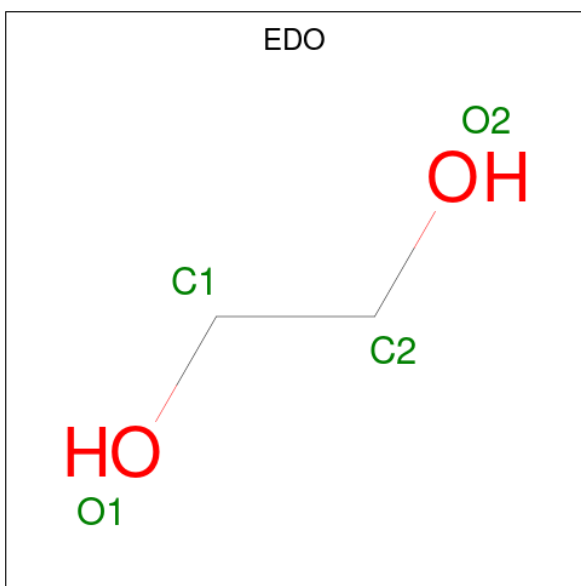
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	H	O	0	0
			10	2	6	2		
8	C	1	Total	C	H	O	0	0
			10	2	6	2		
8	C	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	D	1	Total	C	H	O	0	0
			10	2	6	2		
8	D	1	Total	C	H	O	0	0
			10	2	6	2		
8	D	1	Total	C	H	O	0	0
			10	2	6	2		
8	G	1	Total	C	H	O	0	0
			10	2	6	2		
8	G	1	Total	C	H	O	0	0
			10	2	6	2		

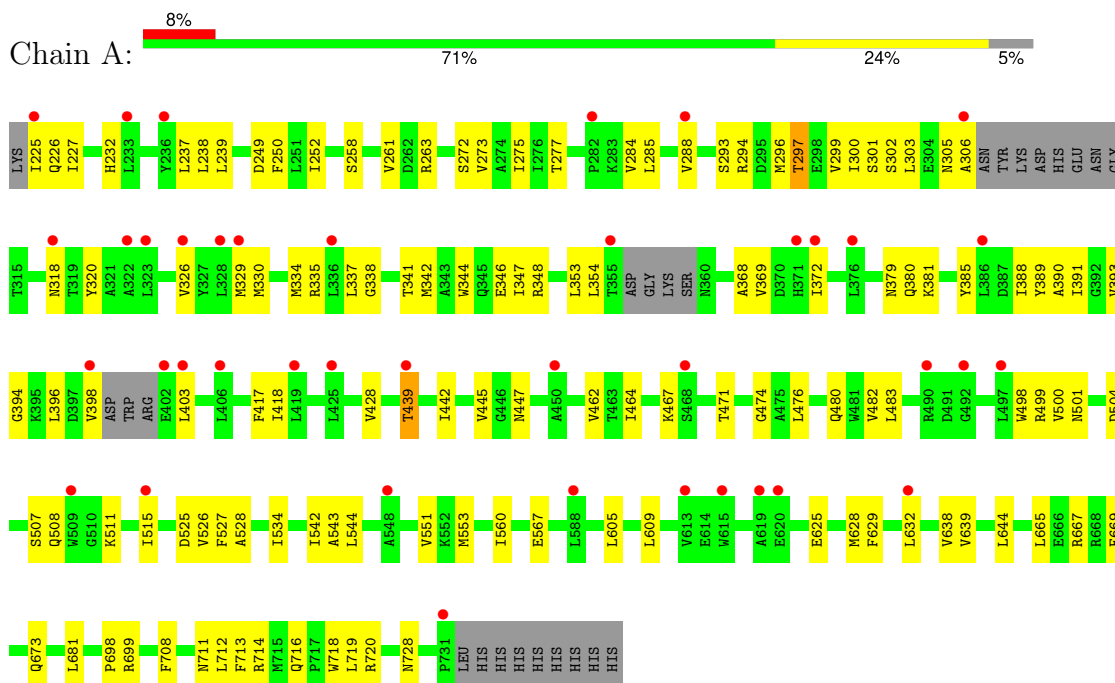
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	O	0	0
			1	1		
9	B	3	Total	O	0	0
			3	3		
9	C	36	Total	O	0	0
			36	36		
9	D	39	Total	O	0	0
			39	39		
9	G	47	Total	O	0	0
			47	47		
9	I	17	Total	O	0	0
			17	17		

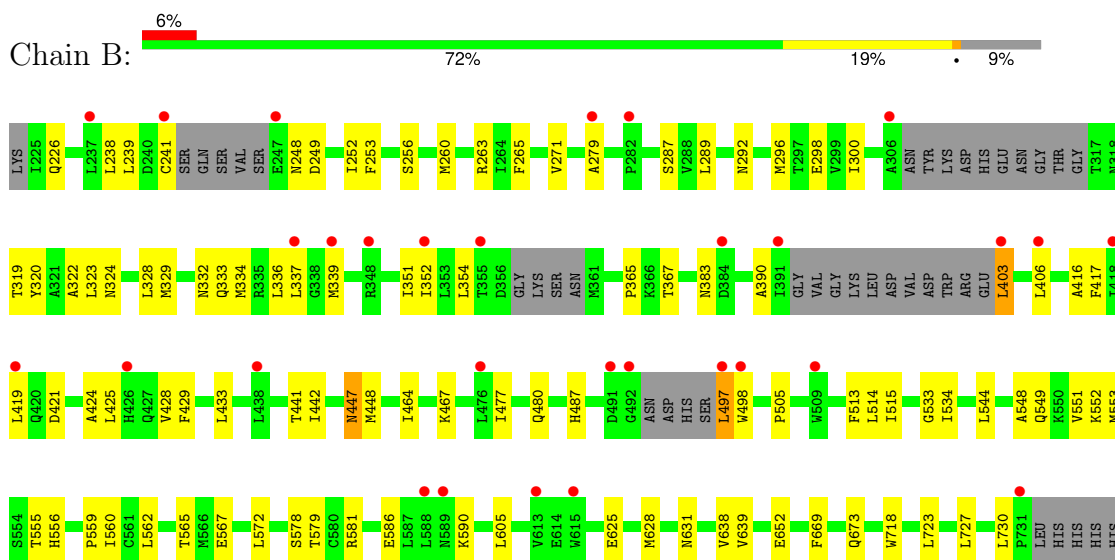
3 Residue-property plots

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: Serine protease complement C2b

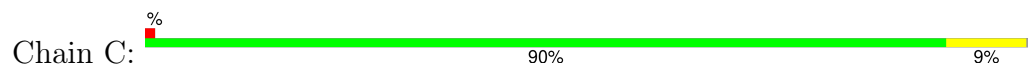


• Molecule 1: Serine protease complement C2b

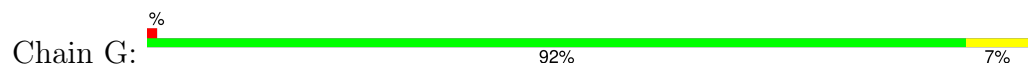




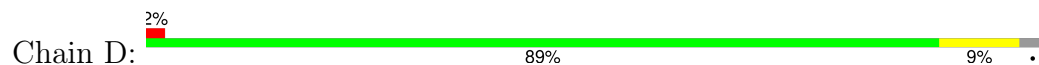
- Molecule 2: Fab light chain



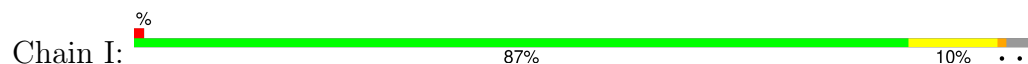
- Molecule 2: Fab light chain



- Molecule 3: Fab heavy chain



- Molecule 3: Fab heavy chain



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



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



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  50% 50%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.24Å 67.79Å 155.37Å 98.32° 90.68° 101.20°	Depositor
Resolution (Å)	48.63 – 2.60 48.63 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.1 (48.63-2.60) 94.1 (48.63-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.208 , 0.256 0.206 , 0.254	Depositor DCC
R_{free} test set	3375 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å ²)	51.9	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28743	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, BMA, MG, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.15	0/3958	0.37	0/5348
1	B	0.14	0/3822	0.36	0/5161
2	C	0.12	0/1628	0.33	0/2221
2	G	0.13	0/1637	0.34	0/2233
3	D	0.15	0/1751	0.37	0/2384
3	I	0.12	0/1758	0.36	0/2394
All	All	0.14	0/14554	0.36	0/19741

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	439	THR	Peptide

5.2 Too-close contacts [i](#)

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	3884	3857	3850	120	0
1	B	3751	3731	3723	91	0
2	C	1591	1548	1548	10	0
2	G	1600	1559	1559	8	0
3	D	1705	1654	1654	15	0
3	I	1705	1654	1645	17	0
4	E	39	34	34	0	0
4	H	39	34	34	3	0
5	F	28	25	25	1	0
5	J	28	25	25	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	B	14	13	13	2	0
8	C	12	18	18	0	0
8	D	12	18	18	1	0
8	G	8	12	12	0	0
9	A	1	0	0	0	0
9	B	3	0	0	0	0
9	C	36	0	0	0	0
9	D	39	0	0	0	0
9	G	47	0	0	1	0
9	I	17	0	0	0	0
All	All	14561	14182	14158	257	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (257) 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:296:MET:CE	1:A:300:ILE:HD11	1.84	1.07
1:A:330:MET:HE1	1:A:372:ILE:HG23	1.37	1.03
1:B:605:LEU:HD13	5:J:2:NAG:H82	1.50	0.93
1:A:534:ILE:HD13	1:A:638:VAL:HG12	1.54	0.90
1:B:334:MET:HE2	1:B:339:MET:SD	2.12	0.88
1:A:296:MET:SD	1:A:300:ILE:HD13	2.16	0.86
1:A:296:MET:HE1	1:A:300:ILE:HD11	1.57	0.85
1:B:555:THR:HG23	1:B:556:HIS:CD2	2.14	0.81
1:B:498:TRP:CE3	1:B:515:ILE:HD11	2.15	0.81
1:B:548:ALA:HB3	1:B:549:GLN:OE1	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:LEU:HD12	1:B:718:TRP:CH2	2.17	0.80
1:A:296:MET:CE	1:A:300:ILE:CD1	2.60	0.78
1:A:296:MET:HE2	1:A:300:ILE:HD11	1.65	0.75
1:B:605:LEU:HD12	1:B:652:GLU:HG3	1.68	0.75
1:A:605:LEU:HD22	5:F:2:NAG:H82	1.68	0.74
1:A:526:VAL:HG13	1:A:527:PHE:CD1	2.24	0.73
1:B:605:LEU:CD1	5:J:2:NAG:H82	2.18	0.73
1:A:273:VAL:HG21	1:A:299:VAL:HG11	1.71	0.72
3:I:3:GLU:O	3:I:4:VAL:HG12	1.91	0.70
1:B:417:PHE:CD1	1:B:428:VAL:HG11	2.27	0.70
1:A:225:ILE:HD11	1:A:389:TYR:CE1	2.28	0.68
1:B:549:GLN:OE1	1:B:549:GLN:N	2.27	0.68
1:A:296:MET:SD	1:A:300:ILE:CD1	2.81	0.68
3:D:50:MET:HE1	3:D:83:LEU:HD21	1.75	0.68
1:B:332:ASN:O	1:B:336:LEU:HD13	1.95	0.67
3:D:122:MET:HE2	8:D:303:EDO:H12	1.77	0.66
3:D:3:GLU:N	3:D:3:GLU:OE1	2.29	0.66
1:A:498:TRP:O	1:A:515:ILE:HD13	1.96	0.65
1:B:351:ILE:C	1:B:352:ILE:HD12	2.21	0.65
1:B:533:GLY:C	1:B:534:ILE:HD12	2.21	0.65
1:B:477:ILE:C	1:B:477:ILE:HD12	2.22	0.65
1:A:297:THR:H	1:A:300:ILE:CD1	2.10	0.64
1:B:417:PHE:CE1	1:B:428:VAL:HG11	2.32	0.64
1:A:226:GLN:C	1:A:227:ILE:HD13	2.23	0.64
1:B:572:LEU:HD22	1:B:586:GLU:OE2	1.99	0.64
1:B:723:LEU:HD13	1:B:727:LEU:HD11	1.81	0.63
1:A:225:ILE:N	1:A:225:ILE:HD12	2.14	0.62
1:B:296:MET:O	1:B:300:ILE:HD12	1.98	0.62
3:I:104:LEU:HD23	3:I:105:LEU:HD23	1.80	0.62
1:B:572:LEU:CD2	1:B:586:GLU:OE2	2.48	0.62
1:A:526:VAL:HG13	1:A:527:PHE:CE1	2.35	0.62
1:A:297:THR:H	1:A:300:ILE:HD12	1.65	0.61
1:B:567:GLU:N	1:B:567:GLU:OE1	2.32	0.61
3:I:177:VAL:HG22	3:I:196:VAL:HG12	1.81	0.61
1:A:467:LYS:HD3	1:A:467:LYS:C	2.25	0.61
1:A:301:SER:O	1:A:305:ASN:OD1	2.18	0.60
1:B:429:PHE:CE1	1:B:433:LEU:HD21	2.36	0.60
1:A:239:LEU:HD22	1:A:354:LEU:HD12	1.82	0.60
3:D:155:LEU:HD21	3:D:157:LYS:HD3	1.84	0.60
1:A:296:MET:HG3	1:A:297:THR:HG23	1.83	0.59
1:B:333:GLN:O	1:B:337:LEU:HD22	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:ALA:O	1:B:428:VAL:HG23	2.02	0.59
1:A:393:VAL:C	1:A:396:LEU:HD21	2.28	0.59
1:A:504:ASP:HB3	1:A:511:LYS:HD3	1.85	0.58
1:A:263:ARG:HD2	1:A:669:PHE:CD2	2.39	0.58
3:I:164:VAL:CG2	3:I:192:LEU:HD21	2.33	0.58
1:B:265:PHE:CE1	1:B:271:VAL:HG13	2.39	0.58
1:A:393:VAL:O	1:A:396:LEU:HD21	2.04	0.57
1:A:249:ASP:HA	1:A:252:ILE:HD13	1.86	0.57
1:B:555:THR:HG23	1:B:556:HIS:NE2	2.20	0.57
1:A:698:PRO:HG2	3:I:32:THR:HG23	1.87	0.57
1:A:560:ILE:HD13	1:A:673:GLN:HB2	1.87	0.57
1:B:638:VAL:HG23	1:B:639:VAL:HG23	1.86	0.57
1:B:406:LEU:HD12	1:B:406:LEU:H	1.70	0.56
1:A:335:ARG:NE	1:A:335:ARG:HA	2.20	0.56
3:I:20:LEU:HD12	3:I:21:LYS:H	1.70	0.56
3:I:143:ARG:HD3	3:I:144:SER:H	1.71	0.56
1:A:296:MET:C	1:A:297:THR:HG23	2.31	0.55
1:A:273:VAL:HG21	1:A:299:VAL:CG1	2.35	0.55
3:I:22:ILE:HD11	3:I:83:LEU:HD23	1.89	0.55
1:B:239:LEU:HG	1:B:354:LEU:HD12	1.89	0.55
4:H:2:NAG:H3	4:H:2:NAG:H83	1.90	0.55
1:A:628:MET:CE	3:I:105:LEU:HD22	2.37	0.54
1:A:498:TRP:C	1:A:499:ARG:HD3	2.32	0.54
1:A:252:ILE:HD12	1:A:252:ILE:N	2.23	0.54
1:B:498:TRP:HE3	1:B:515:ILE:HD11	1.71	0.54
1:B:605:LEU:HD12	1:B:652:GLU:CG	2.37	0.54
3:I:164:VAL:HG23	3:I:192:LEU:HD21	1.90	0.54
1:B:515:ILE:O	1:B:515:ILE:HD12	2.07	0.53
1:B:625:GLU:OE2	1:B:628:MET:HG3	2.08	0.53
1:A:320:TYR:CD1	1:A:320:TYR:C	2.87	0.53
3:I:192:LEU:C	3:I:192:LEU:HD12	2.34	0.53
1:A:498:TRP:C	1:A:515:ILE:HD13	2.33	0.53
1:A:718:TRP:CZ3	1:A:719:LEU:HD23	2.44	0.53
1:A:369:VAL:HA	1:A:372:ILE:HG12	1.91	0.53
1:A:628:MET:HE1	1:A:681:LEU:O	2.08	0.53
1:A:318:ASN:OD1	1:A:318:ASN:C	2.53	0.53
1:A:628:MET:HE2	3:I:105:LEU:HD22	1.90	0.52
1:B:383:ASN:OD1	1:B:383:ASN:O	2.27	0.52
1:A:294:ARG:HG3	1:A:294:ARG:HH11	1.73	0.52
1:B:581:ARG:O	1:B:581:ARG:HD3	2.10	0.52
1:B:421:ASP:OD1	1:B:421:ASP:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:560:ILE:HD13	1:B:673:GLN:HB2	1.90	0.52
1:A:335:ARG:HA	1:A:335:ARG:HE	1.75	0.52
1:A:342:MET:HE3	1:A:346:GLU:OE2	2.10	0.51
2:C:40:LEU:HD13	2:C:85:ALA:HB2	1.91	0.51
1:A:239:LEU:CD2	1:A:354:LEU:HD12	2.41	0.51
1:B:505:PRO:HA	1:B:556:HIS:CE1	2.45	0.51
1:A:380:GLN:HG3	1:A:381:LYS:N	2.25	0.51
1:B:417:PHE:CE1	1:B:428:VAL:CG1	2.93	0.51
3:D:155:LEU:HG	3:D:157:LYS:HG2	1.91	0.51
1:A:711:ASN:OD1	1:A:714:ARG:HG2	2.11	0.51
1:B:265:PHE:CD2	1:B:296:MET:HG3	2.46	0.51
1:B:534:ILE:HD12	1:B:534:ILE:N	2.25	0.51
1:A:226:GLN:O	1:A:227:ILE:HD13	2.10	0.50
1:A:284:VAL:HG23	1:A:284:VAL:O	2.10	0.50
1:B:319:THR:O	1:B:323:LEU:HD12	2.11	0.50
1:B:480:GLN:CG	1:B:480:GLN:O	2.58	0.50
2:C:19:THR:HG21	9:G:407:HOH:O	2.11	0.50
1:A:544:LEU:HD12	1:A:718:TRP:CH2	2.46	0.50
1:A:326:VAL:O	1:A:330:MET:HG3	2.12	0.50
1:B:467:LYS:HG2	1:B:497:LEU:HD22	1.94	0.50
1:B:447:ASN:OD1	4:H:1:NAG:C1	2.60	0.49
1:B:324:ASN:O	1:B:328:LEU:HG	2.13	0.49
1:A:638:VAL:HG23	1:A:639:VAL:HG23	1.94	0.49
1:A:232:HIS:NE2	1:A:272:SER:OG	2.45	0.49
1:A:334:MET:HG3	1:A:344:TRP:CE2	2.47	0.49
1:A:699:ARG:H	1:A:699:ARG:HD3	1.78	0.49
1:B:514:LEU:HD12	1:B:514:LEU:N	2.28	0.49
1:A:346:GLU:HA	1:A:385:TYR:OH	2.13	0.49
3:I:102:SER:HB3	3:I:110:PRO:O	2.12	0.49
1:A:394:GLY:C	1:A:396:LEU:HD22	2.38	0.48
3:D:164:VAL:HG23	3:D:192:LEU:HD21	1.94	0.48
1:A:388:ILE:HG13	1:A:388:ILE:O	2.13	0.48
1:B:631:ASN:OD1	7:B:801:NAG:O5	2.27	0.48
1:A:379:ASN:OD1	1:A:381:LYS:N	2.47	0.48
1:B:723:LEU:HB3	1:B:727:LEU:CD1	2.43	0.48
1:A:368:ALA:O	1:A:372:ILE:HG12	2.13	0.48
1:A:716:GLN:O	1:A:720:ARG:HG2	2.14	0.48
2:C:19:THR:HG23	2:C:73:SER:OG	2.13	0.48
1:A:500:VAL:HG23	1:A:515:ILE:HD11	1.96	0.48
1:B:253:PHE:CD1	1:B:354:LEU:HB3	2.49	0.48
1:B:505:PRO:HD2	1:B:552:LYS:HE2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:PHE:HZ	1:A:306:ALA:HB1	1.79	0.47
1:B:260:MET:HE1	1:B:352:ILE:HG21	1.94	0.47
1:A:499:ARG:HD3	1:A:499:ARG:N	2.29	0.47
1:B:260:MET:HE2	1:B:429:PHE:HE2	1.79	0.47
1:A:232:HIS:CE1	1:A:294:ARG:HE	2.32	0.47
1:A:342:MET:HE3	1:A:346:GLU:CD	2.39	0.47
3:D:166:VAL:HG11	3:D:194:SER:CB	2.44	0.47
1:B:590:LYS:N	1:B:590:LYS:HD3	2.29	0.47
2:G:96:LEU:HD12	2:G:100:ILE:HD11	1.97	0.47
1:A:337:LEU:HD12	1:A:337:LEU:N	2.30	0.47
1:A:398:VAL:HG11	1:A:418:ILE:HG12	1.97	0.47
1:A:483:LEU:HD11	1:A:542:ILE:HD11	1.96	0.47
3:I:6:LEU:HD23	3:I:26:GLY:HA2	1.97	0.47
1:A:609:LEU:HD22	1:A:644:LEU:HB3	1.97	0.47
1:A:625:GLU:HG3	1:A:628:MET:HE3	1.96	0.47
1:A:342:MET:O	1:A:346:GLU:HG2	2.16	0.46
1:A:467:LYS:C	1:A:467:LYS:CD	2.88	0.46
1:B:260:MET:HE2	1:B:429:PHE:CE2	2.51	0.46
1:B:553:MET:SD	1:B:559:PRO:HD3	2.56	0.46
3:D:192:LEU:C	3:D:192:LEU:HD12	2.39	0.46
3:D:50:MET:CE	3:D:83:LEU:HD21	2.45	0.46
1:A:275:ILE:HD12	1:A:303:LEU:HD13	1.96	0.46
1:A:718:TRP:HZ3	1:A:719:LEU:HD23	1.81	0.46
1:B:464:ILE:HD13	1:B:464:ILE:N	2.31	0.46
1:A:302:SER:HA	1:A:305:ASN:ND2	2.29	0.46
1:A:504:ASP:CB	1:A:511:LYS:HD3	2.45	0.46
1:B:265:PHE:HE1	1:B:271:VAL:HG13	1.77	0.46
1:B:578:SER:O	1:B:730:LEU:HD13	2.16	0.46
3:D:164:VAL:CG2	3:D:192:LEU:HD21	2.46	0.46
2:C:214:GLU:OE1	3:D:142:SER:HB3	2.16	0.46
3:D:95:MET:HE2	3:D:95:MET:HB2	1.87	0.46
2:C:164:GLU:OE2	3:D:185:GLN:HA	2.16	0.46
1:A:639:VAL:HG21	1:A:708:PHE:CE1	2.52	0.45
1:B:253:PHE:CE1	1:B:354:LEU:HB3	2.51	0.45
1:A:525:ASP:OD2	1:A:528:ALA:HB2	2.16	0.45
1:A:237:LEU:C	1:A:238:LEU:HD12	2.42	0.45
1:A:553:MET:N	1:A:553:MET:HE2	2.31	0.45
1:B:447:ASN:HD21	4:H:1:NAG:C1	2.30	0.45
1:B:590:LYS:HD3	1:B:590:LYS:H	1.80	0.45
1:B:467:LYS:HG3	1:B:497:LEU:HD13	2.00	0.44
3:D:173:LEU:HD21	3:D:196:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:51:GLU:O	2:C:52:ASP:HB2	2.18	0.44
1:A:467:LYS:CD	1:A:467:LYS:O	2.65	0.44
1:A:665:LEU:HD13	1:A:667:ARG:NH1	2.32	0.44
1:B:515:ILE:HD12	1:B:515:ILE:C	2.43	0.44
1:B:292:ASN:OD1	1:B:298:GLU:CD	2.61	0.44
1:A:232:HIS:HB3	1:A:347:ILE:HG22	2.00	0.44
1:A:398:VAL:HG11	1:A:418:ILE:CG1	2.48	0.44
2:G:121:LEU:HD21	2:G:210:VAL:HG22	2.00	0.44
1:A:258:SER:HA	1:A:261:VAL:HG12	1.99	0.43
1:B:562:LEU:O	1:B:565:THR:HG22	2.18	0.43
2:C:43:THR:HG22	2:C:44:ALA:N	2.32	0.43
1:B:333:GLN:O	1:B:337:LEU:CD2	2.66	0.43
1:B:487:HIS:C	1:B:487:HIS:CD2	2.95	0.43
1:A:272:SER:OG	1:A:294:ARG:CZ	2.67	0.43
1:A:629:PHE:CG	1:A:632:LEU:HD22	2.54	0.43
1:B:300:ILE:HD12	1:B:300:ILE:H	1.82	0.43
1:A:354:LEU:HD23	1:A:391:ILE:HB	2.00	0.43
2:G:43:THR:HG22	2:G:44:ALA:N	2.34	0.43
1:A:273:VAL:HG21	1:A:299:VAL:HG21	2.00	0.43
1:A:379:ASN:OD1	1:A:379:ASN:C	2.61	0.43
1:A:273:VAL:O	1:A:293:SER:HB2	2.18	0.43
1:A:296:MET:O	1:A:297:THR:HG23	2.18	0.43
1:A:348:ARG:HG3	1:A:385:TYR:CD1	2.53	0.43
1:B:419:LEU:HD11	1:B:428:VAL:HG21	2.00	0.43
1:A:277:THR:HG23	1:A:285:LEU:CD2	2.49	0.43
1:A:480:GLN:O	1:A:480:GLN:HG2	2.19	0.43
1:A:238:LEU:C	1:A:239:LEU:HD23	2.44	0.43
1:A:507:SER:O	1:A:508:GLN:HB3	2.19	0.43
1:B:565:THR:OG1	1:B:567:GLU:OE1	2.29	0.42
3:D:215:LYS:N	3:D:216:PRO:CD	2.82	0.42
1:A:288:VAL:H	1:A:329:MET:HE1	1.84	0.42
1:A:390:ALA:HB3	1:A:403:LEU:HD21	2.01	0.42
2:G:62:ARG:HD2	2:G:77:SER:O	2.19	0.42
3:I:142:SER:O	3:I:143:ARG:HB3	2.19	0.42
1:A:417:PHE:CD2	1:A:428:VAL:HG21	2.54	0.42
1:A:699:ARG:HD3	1:A:699:ARG:N	2.35	0.42
1:B:241:CYS:HB2	1:B:279:ALA:HB2	2.01	0.42
1:B:263:ARG:HD3	1:B:669:PHE:CD2	2.54	0.42
1:A:462:VAL:HG22	1:A:474:GLY:C	2.45	0.42
1:A:483:LEU:HD21	1:A:712:LEU:HD21	2.02	0.42
1:B:289:LEU:HD22	1:B:336:LEU:CD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:ILE:HD13	1:A:445:VAL:HG21	2.02	0.42
1:B:390:ALA:HB1	1:B:403:LEU:HD23	2.01	0.42
1:B:551:VAL:HG13	1:B:553:MET:CE	2.49	0.42
2:C:136:LEU:HD13	2:C:182:LEU:HD23	2.01	0.42
2:G:35:LYS:HG3	2:G:50:TYR:HA	2.02	0.41
1:A:288:VAL:H	1:A:329:MET:CE	2.33	0.41
1:A:294:ARG:HG3	1:A:294:ARG:NH1	2.35	0.41
2:C:140:ILE:HG12	2:C:199:VAL:HG21	2.01	0.41
2:G:136:LEU:N	2:G:136:LEU:HD12	2.35	0.41
1:A:499:ARG:N	1:A:499:ARG:CD	2.82	0.41
1:A:525:ASP:CG	1:A:528:ALA:HB2	2.46	0.41
1:B:226:GLN:N	1:B:226:GLN:OE1	2.53	0.41
1:B:287:SER:HA	1:B:329:MET:HE1	2.02	0.41
1:B:567:GLU:N	1:B:567:GLU:CD	2.77	0.41
1:A:296:MET:HE1	1:A:300:ILE:CD1	2.38	0.41
1:A:711:ASN:HD21	1:A:713:PHE:HD2	1.68	0.41
2:C:60:PRO:HB2	2:C:62:ARG:HG2	2.02	0.41
3:I:33:SER:HB3	3:I:104:LEU:HD13	2.01	0.41
1:B:320:TYR:CE1	1:B:367:THR:HB	2.56	0.41
1:A:338:GLY:CA	1:A:341:THR:HG22	2.51	0.41
1:A:464:ILE:N	1:A:464:ILE:HD12	2.36	0.41
1:B:416:ALA:C	1:B:417:PHE:CD2	2.99	0.41
1:A:669:PHE:N	1:A:669:PHE:CD1	2.89	0.41
1:B:467:LYS:CG	1:B:497:LEU:HD13	2.50	0.41
1:B:631:ASN:OD1	7:B:801:NAG:C2	2.60	0.41
2:G:112:GLN:HG2	2:G:144:TYR:CZ	2.56	0.41
1:B:448:MET:SD	1:B:448:MET:N	2.93	0.41
2:G:51:GLU:O	2:G:52:ASP:HB2	2.20	0.41
1:A:567:GLU:OE2	1:A:728:ASN:OD1	2.39	0.40
1:B:248:ASN:OD1	1:B:249:ASP:N	2.54	0.40
1:B:248:ASN:O	1:B:252:ILE:HG12	2.21	0.40
1:B:323:LEU:CD1	1:B:365:PRO:HB3	2.51	0.40
1:B:441:THR:O	1:B:442:ILE:C	2.63	0.40
1:A:483:LEU:HD12	1:A:543:ALA:O	2.20	0.40
1:B:513:PHE:CE2	1:B:551:VAL:HG23	2.55	0.40
1:B:544:LEU:HD22	1:B:723:LEU:HD21	2.03	0.40
1:A:476:LEU:HD23	1:A:482:VAL:HG22	2.03	0.40
1:B:238:LEU:HD23	1:B:322:ALA:HB1	2.03	0.40
1:A:527:PHE:CD1	1:A:527:PHE:N	2.87	0.40
1:A:238:LEU:HD22	1:A:353:LEU:HD11	2.03	0.40
1:B:256:SER:HB3	1:B:425:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:14:LYS:O	3:I:125:VAL:HA	2.21	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	484/517 (94%)	442 (91%)	41 (8%)	1 (0%)	43	66
1	B	461/517 (89%)	420 (91%)	41 (9%)	0	100	100
2	C	212/216 (98%)	204 (96%)	8 (4%)	0	100	100
2	G	213/216 (99%)	207 (97%)	6 (3%)	0	100	100
3	D	223/231 (96%)	215 (96%)	8 (4%)	0	100	100
3	I	224/231 (97%)	215 (96%)	8 (4%)	1 (0%)	30	51
All	All	1817/1928 (94%)	1703 (94%)	112 (6%)	2 (0%)	48	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	297	THR
3	I	4	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	433/456 (95%)	428 (99%)	5 (1%)	63	83
1	B	417/456 (91%)	413 (99%)	4 (1%)	68	86
2	C	178/180 (99%)	175 (98%)	3 (2%)	53	78
2	G	179/180 (99%)	178 (99%)	1 (1%)	78	91
3	D	192/197 (98%)	189 (98%)	3 (2%)	55	79
3	I	193/197 (98%)	190 (98%)	3 (2%)	55	79
All	All	1592/1666 (96%)	1573 (99%)	19 (1%)	63	83

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	439	THR
1	A	447	ASN
1	A	471	THR
1	A	501	ASN
1	A	551	VAL
1	B	403	LEU
1	B	447	ASN
1	B	497	LEU
1	B	579	THR
2	C	23	SER
2	C	95	SER
2	C	206	VAL
3	D	27	SER
3	D	91	SER
3	D	130	THR
2	G	64	SER
3	I	125	VAL
3	I	141	CYS
3	I	195	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	234	ASN
1	A	349	HIS
1	A	532	GLN
1	A	673	GLN
1	B	232	HIS
1	B	332	ASN

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Mol	Chain	Res	Type
1	B	404	ASN
1	B	608	ASN
2	G	201	HIS
3	I	69	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

10 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	$\# Z > 2$
4	NAG	E	1	4,1	14,14,15	0.80	0	17,19,21	1.48	4 (23%)
4	NAG	E	2	4	14,14,15	0.71	0	17,19,21	0.96	1 (5%)
4	BMA	E	3	4	11,11,12	0.84	0	15,15,17	2.40	5 (33%)
5	NAG	F	1	1,5	14,14,15	0.72	0	17,19,21	1.28	2 (11%)
5	NAG	F	2	5	14,14,15	0.68	0	17,19,21	1.03	1 (5%)
4	NAG	H	1	4	14,14,15	0.95	1 (7%)	17,19,21	1.27	1 (5%)
4	NAG	H	2	4	14,14,15	0.72	0	17,19,21	1.91	3 (17%)
4	BMA	H	3	4	11,11,12	0.79	0	15,15,17	2.52	5 (33%)
5	NAG	J	1	1,5	14,14,15	0.68	0	17,19,21	1.24	2 (11%)
5	NAG	J	2	5	14,14,15	0.63	0	17,19,21	1.36	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
4	NAG	H	1	4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	4/6/23/26	0/1/1/1
4	BMA	H	3	4	-	0/2/19/22	0/1/1/1
5	NAG	J	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	NAG	O5-C1	-2.67	1.39	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	3	BMA	C1-O5-C5	7.99	122.89	112.19
4	E	3	BMA	C1-O5-C5	6.46	120.84	112.19
4	H	2	NAG	C2-N2-C7	5.58	130.38	122.90
4	E	3	BMA	C3-C4-C5	4.02	117.52	110.23
5	J	2	NAG	C1-C2-N2	3.24	115.53	110.43
5	F	1	NAG	C1-C2-N2	-3.18	105.42	110.43
5	J	1	NAG	C1-C2-N2	-3.16	105.45	110.43
4	E	3	BMA	C2-C3-C4	3.00	116.13	110.86
4	E	1	NAG	C2-N2-C7	2.84	126.70	122.90
5	F	1	NAG	O5-C1-C2	-2.83	106.92	111.29
4	H	1	NAG	C1-O5-C5	-2.79	108.45	112.19
4	H	2	NAG	C1-C2-N2	2.76	114.78	110.43
4	H	2	NAG	C1-O5-C5	2.67	115.77	112.19
4	E	2	NAG	C1-O5-C5	2.62	115.69	112.19
4	H	3	BMA	C3-C4-C5	2.58	114.91	110.23
5	J	1	NAG	O5-C1-C2	-2.54	107.37	111.29
4	E	3	BMA	O4-C4-C3	-2.53	104.41	110.38
4	E	1	NAG	O5-C1-C2	-2.53	107.38	111.29
4	E	1	NAG	C4-C3-C2	2.36	114.47	111.02
5	J	2	NAG	C1-O5-C5	2.32	115.29	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	2	NAG	O5-C1-C2	-2.31	107.72	111.29
4	H	3	BMA	O4-C4-C3	-2.19	105.20	110.38
5	F	2	NAG	C1-C2-N2	2.19	113.88	110.43
4	H	3	BMA	C2-C3-C4	2.13	114.61	110.86
4	E	3	BMA	O5-C5-C4	2.10	115.93	110.83
4	H	3	BMA	O3-C3-C2	-2.06	105.84	110.05
4	E	1	NAG	C8-C7-N2	-2.00	112.80	116.12

There are no chirality outliers.

All (8) torsion outliers are listed below:

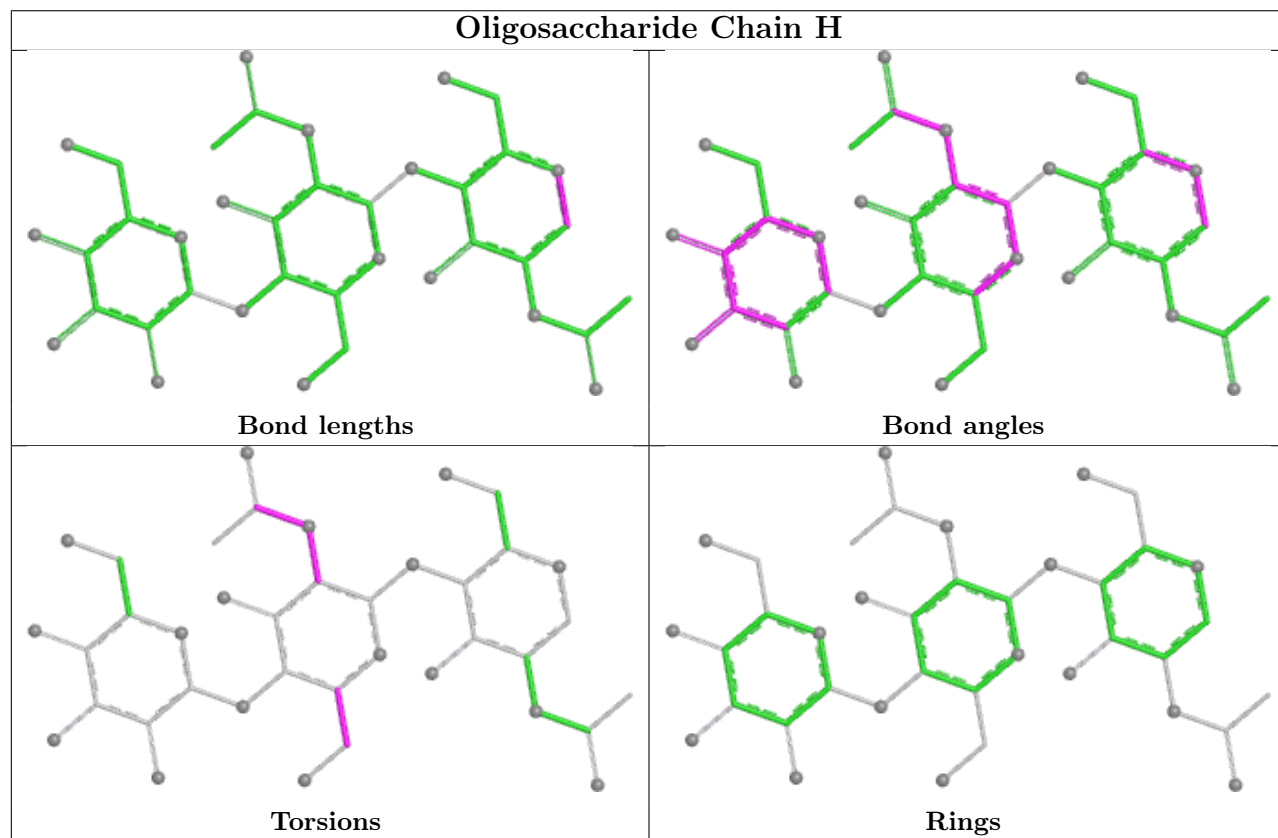
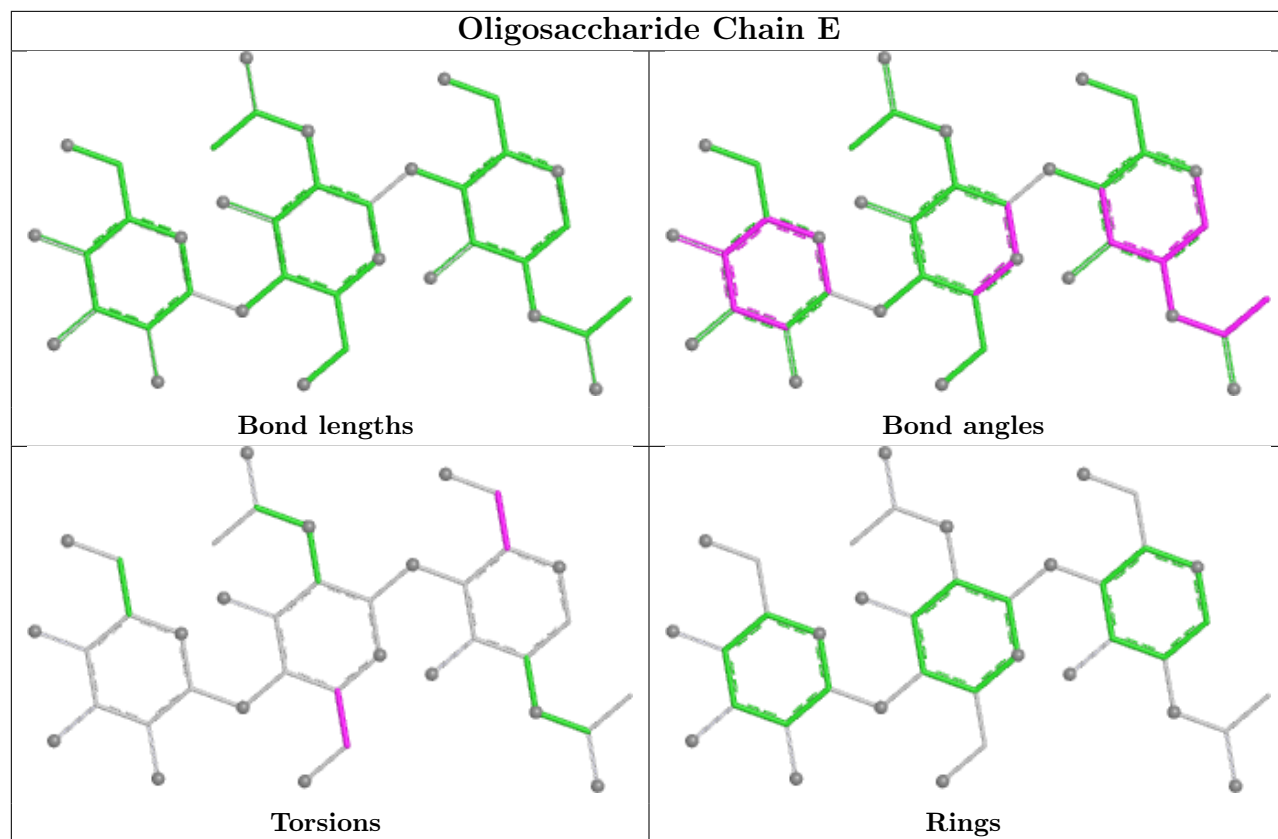
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	H	2	NAG	C8-C7-N2-C2
4	H	2	NAG	O7-C7-N2-C2
4	E	2	NAG	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
4	H	2	NAG	C3-C2-N2-C7
4	E	2	NAG	C4-C5-C6-O6

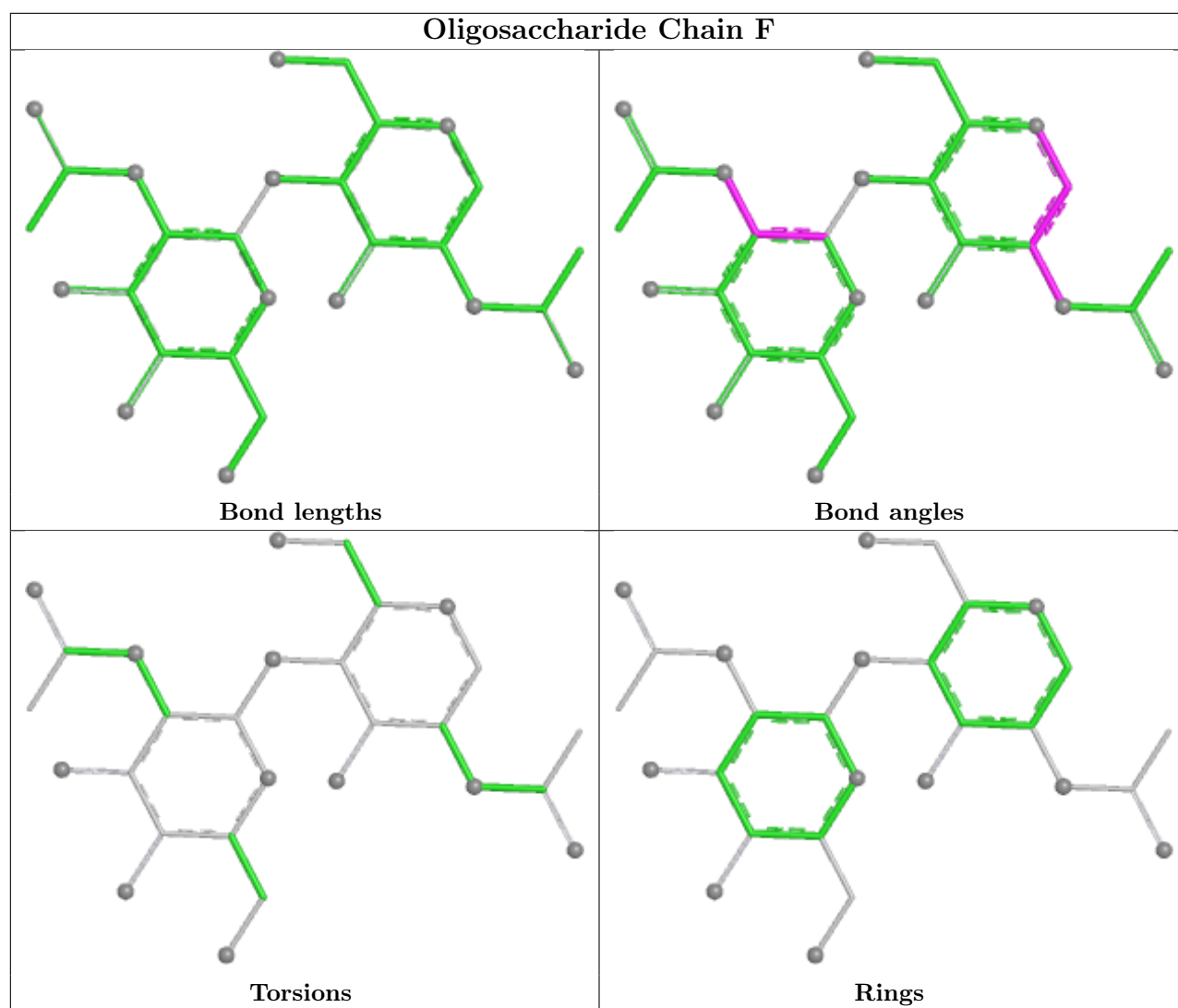
There are no ring outliers.

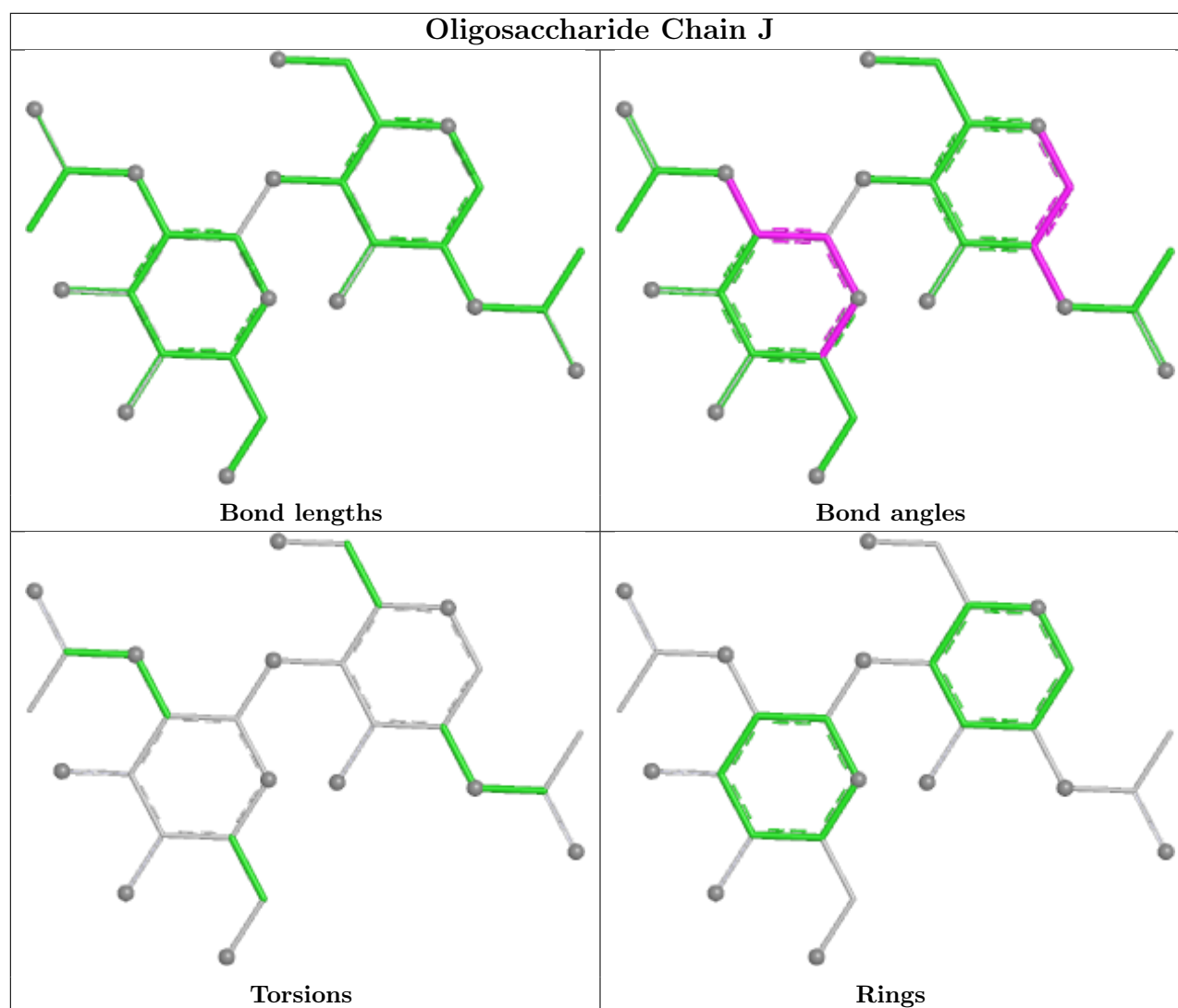
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	2	NAG	1	0
4	H	1	NAG	2	0
5	J	2	NAG	2	0
5	F	2	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 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	EDO	C	303	-	3,3,3	0.25	0	2,2,2	0.31	0
7	NAG	B	801	1	14,14,15	1.30	2 (14%)	17,19,21	1.89	6 (35%)
8	EDO	G	302	-	3,3,3	0.25	0	2,2,2	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	EDO	D	301	-	3,3,3	0.26	0	2,2,2	0.26	0
8	EDO	D	302	-	3,3,3	0.26	0	2,2,2	0.25	0
8	EDO	C	301	-	3,3,3	0.25	0	2,2,2	0.36	0
8	EDO	D	303	-	3,3,3	0.28	0	2,2,2	0.25	0
8	EDO	G	301	-	3,3,3	0.24	0	2,2,2	0.32	0
8	EDO	C	302	-	3,3,3	0.26	0	2,2,2	0.32	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
8	EDO	C	303	-	-	1/1/1/1	-
7	NAG	B	801	1	-	0/6/23/26	0/1/1/1
8	EDO	G	302	-	-	0/1/1/1	-
8	EDO	D	301	-	-	0/1/1/1	-
8	EDO	D	302	-	-	0/1/1/1	-
8	EDO	C	301	-	-	0/1/1/1	-
8	EDO	D	303	-	-	1/1/1/1	-
8	EDO	G	301	-	-	0/1/1/1	-
8	EDO	C	302	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	801	NAG	C1-C2	3.80	1.57	1.52
7	B	801	NAG	O5-C1	2.23	1.47	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	801	NAG	O5-C1-C2	-3.64	105.66	111.29
7	B	801	NAG	O5-C5-C6	3.59	114.66	107.66
7	B	801	NAG	C4-C3-C2	-2.71	107.05	111.02
7	B	801	NAG	C1-C2-N2	-2.45	106.58	110.43
7	B	801	NAG	C1-O5-C5	-2.37	109.00	112.19
7	B	801	NAG	C2-N2-C7	2.37	126.08	122.90

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	302	EDO	O1-C1-C2-O2
8	C	303	EDO	O1-C1-C2-O2
8	D	303	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	801	NAG	2	0
8	D	303	EDO	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

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	492/517 (95%)	0.80	40 (8%)	18 14	56, 118, 160, 190	0
1	B	473/517 (91%)	0.70	30 (6%)	26 20	51, 112, 160, 198	0
2	C	214/216 (99%)	-0.12	2 (0%)	81 78	35, 56, 105, 128	0
2	G	215/216 (99%)	-0.27	2 (0%)	81 78	37, 50, 73, 127	0
3	D	225/231 (97%)	-0.25	4 (1%)	67 63	41, 53, 80, 159	0
3	I	225/231 (97%)	-0.11	2 (0%)	81 78	40, 61, 105, 147	0
All	All	1844/1928 (95%)	0.30	80 (4%)	40 34	35, 80, 153, 198	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	492	GLY	5.4
1	B	498	TRP	4.7
1	B	241	CYS	4.6
1	B	731	PRO	4.5
1	A	233	LEU	4.2
1	A	731	PRO	4.1
1	A	406	LEU	3.7
1	B	497	LEU	3.7
1	B	306	ALA	3.7
1	B	615	TRP	3.6
1	B	282	PRO	3.6
2	C	3	VAL	3.6
1	A	306	ALA	3.4
1	A	497	LEU	3.3
1	A	236	TYR	3.3
1	B	348	ARG	3.3
1	A	329	MET	3.2
1	B	438	LEU	3.1
1	A	326	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	398	VAL	3.1
1	A	439	THR	3.0
1	A	632	LEU	2.9
1	B	509	TRP	2.9
1	A	619	ALA	2.9
1	B	403	LEU	2.7
1	A	372	ILE	2.7
1	A	323	LEU	2.6
1	A	371	HIS	2.6
1	B	247	GLU	2.6
1	B	589	ASN	2.6
1	B	339	MET	2.5
1	A	615	TRP	2.5
1	A	490	ARG	2.5
1	A	509	TRP	2.5
1	B	491	ASP	2.4
1	B	384	ASP	2.4
2	G	215	CYS	2.4
1	A	613	VAL	2.4
1	B	588	LEU	2.4
1	A	419	LEU	2.3
1	A	515	ILE	2.3
3	D	145	THR	2.3
1	A	318	ASN	2.3
1	B	279	ALA	2.3
3	D	144	SER	2.3
1	A	288	VAL	2.3
1	A	403	LEU	2.3
1	B	419	LEU	2.3
1	A	282	PRO	2.3
1	A	468	SER	2.3
1	A	492	GLY	2.3
1	A	328	LEU	2.3
1	B	613	VAL	2.3
1	A	322	ALA	2.2
1	B	355	THR	2.2
1	B	476	LEU	2.2
1	A	450	ALA	2.2
1	B	391	ILE	2.2
1	A	425	LEU	2.2
1	B	237	LEU	2.2
1	A	225	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	355	THR	2.2
1	A	402	GLU	2.2
1	B	418	ILE	2.2
1	A	588	LEU	2.2
1	A	548	ALA	2.1
3	I	141	CYS	2.1
1	A	336	LEU	2.1
3	I	140	PRO	2.1
1	A	376	LEU	2.1
1	B	337	LEU	2.1
1	B	406	LEU	2.1
3	D	143	ARG	2.1
1	A	386	LEU	2.1
1	A	620	GLU	2.0
1	B	426	HIS	2.0
1	B	352	ILE	2.0
3	D	3	GLU	2.0
2	G	1	GLN	2.0
2	C	159	VAL	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.

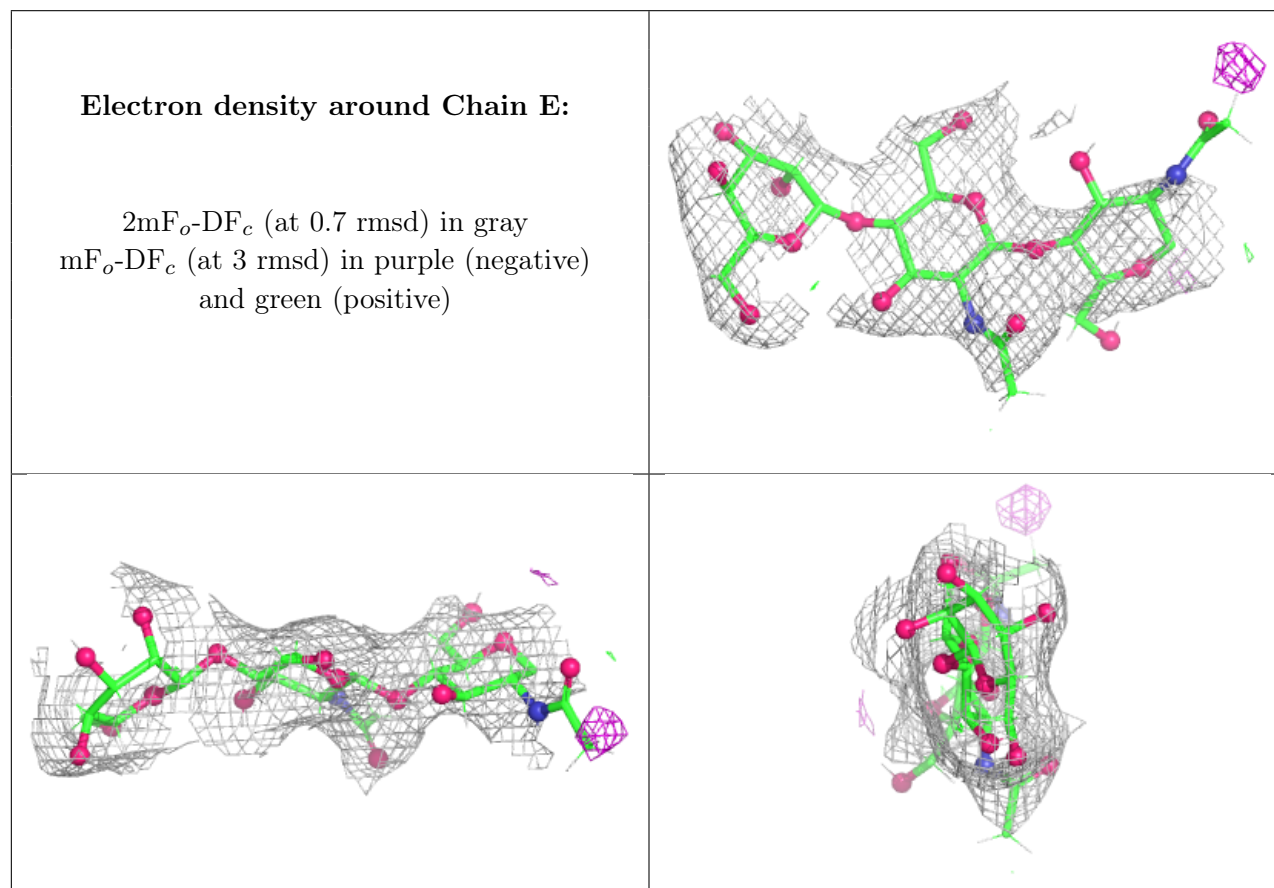
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	E	1	14/15	-	-	154,159,190,193	0
4	NAG	E	2	14/15	-	-	126,141,165,167	0
4	BMA	E	3	11/12	-	-	118,131,154,160	0
4	NAG	H	2	14/15	0.72	0.17	119,131,156,157	0
5	NAG	J	2	14/15	0.72	0.16	108,128,153,154	0
4	BMA	H	3	11/12	-	-	117,122,145,152	0
5	NAG	F	1	14/15	-	-	88,106,121,127	0
5	NAG	F	2	14/15	-	-	146,163,192,202	0
5	NAG	J	1	14/15	0.82	0.15	80,98,115,122	0

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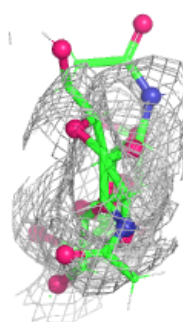
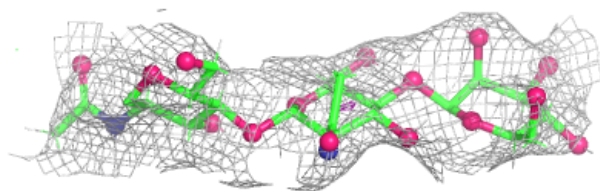
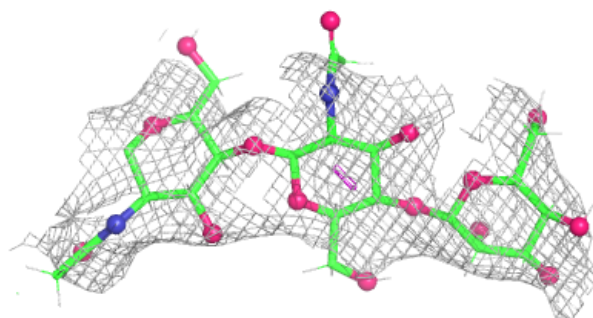
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	H	1	14/15	0.83	0.19	118,132,154,164	0

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.

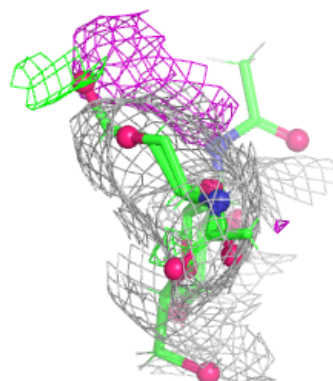
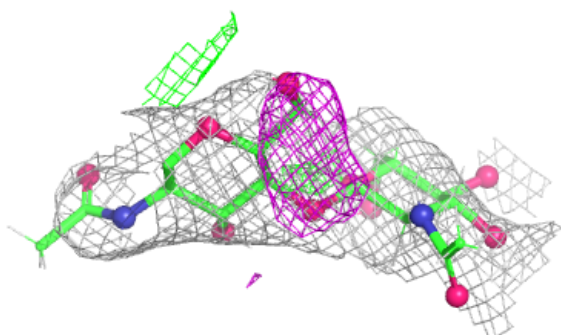
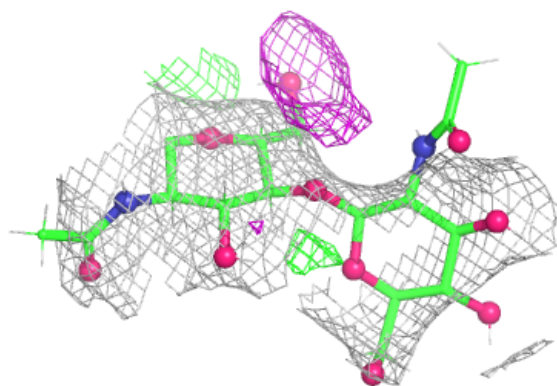


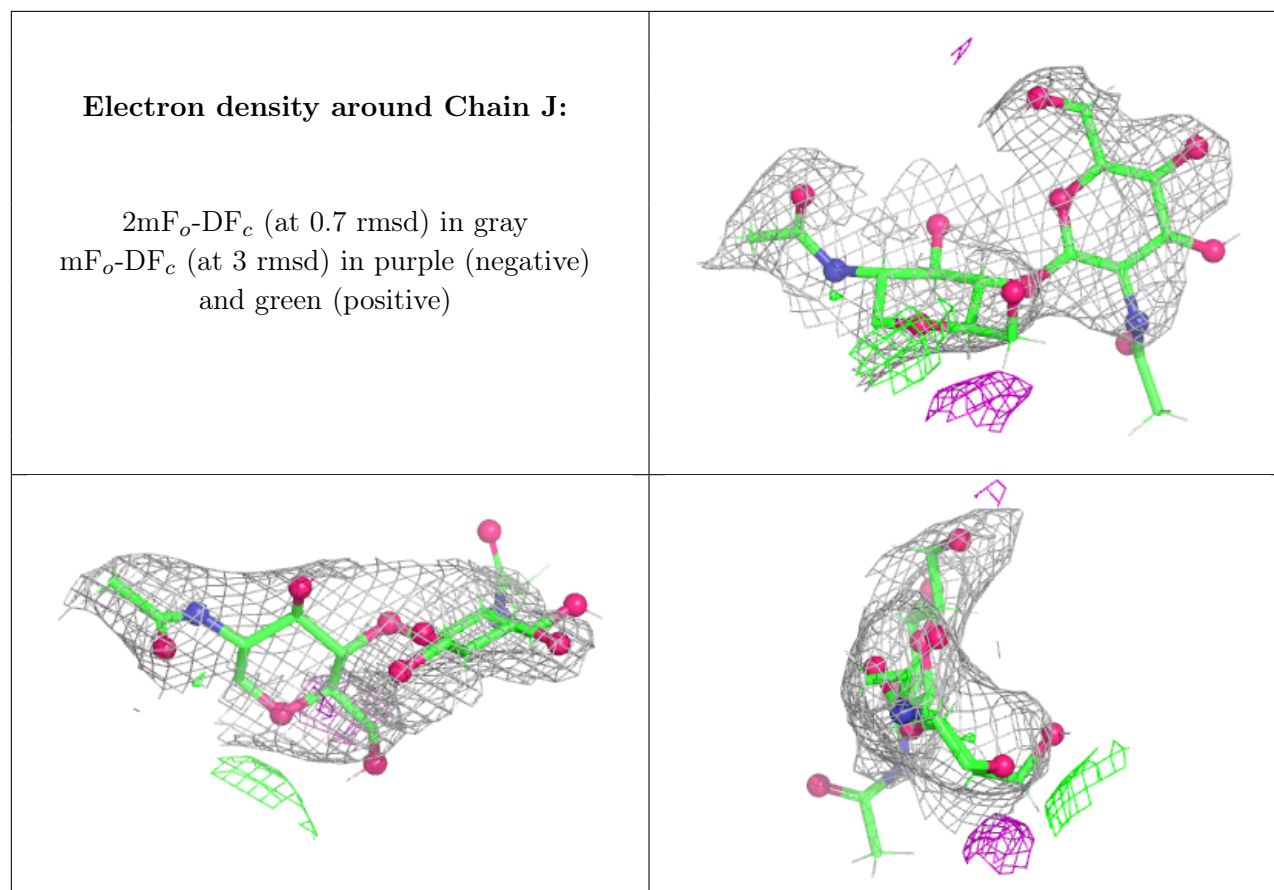
Electron density around Chain H:

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

**Electron density around Chain F:**

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





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	B	801	14/15	0.71	0.11	100,119,134,143	0
8	EDO	C	301	4/4	0.80	0.29	69,83,89,90	0
8	EDO	D	303	4/4	0.83	0.29	90,108,110,110	0
8	EDO	D	302	4/4	0.84	0.22	55,66,76,76	0
8	EDO	D	301	4/4	0.84	0.18	58,69,86,86	0
8	EDO	G	301	4/4	0.86	0.23	74,89,103,103	0
8	EDO	G	302	4/4	0.87	0.15	53,64,73,73	0
8	EDO	C	303	4/4	0.89	0.16	54,65,76,80	0
6	MG	A	801	1/1	0.95	0.10	70,70,70,70	0
8	EDO	C	302	4/4	0.95	0.09	44,52,63,63	0
6	MG	B	802	1/1	0.98	0.04	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.