



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 03:38 AM BST

PDB ID : 1S78  
Title : Insights into ErbB signaling from the structure of the ErbB2-pertuzumab complex  
Authors : Franklin, M.C.; Carey, K.D.; Vajdos, F.F.; Leahy, D.J.; de Vos, A.M.; Sliwkowski, M.X.  
Deposited on : 2004-01-29  
Resolution : 3.25 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

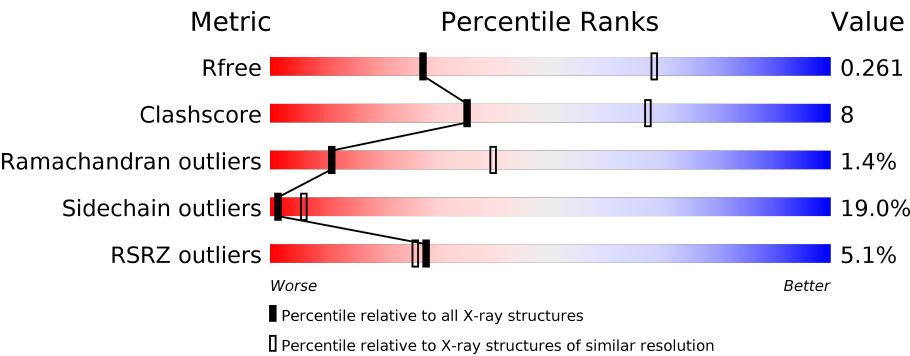
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 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.



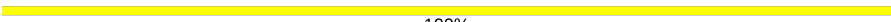
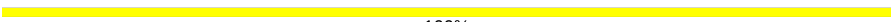
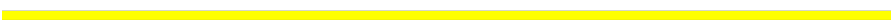

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	624	<div><div>3%</div><div><div></div><div>64%</div><div>21%</div><div>5%</div><div>11%</div></div></div>
1	B	624	<div><div>2%</div><div><div></div><div>63%</div><div>23%</div><div>5%</div><div>9%</div></div></div>
2	C	214	<div><div>16%</div><div><div></div><div>60%</div><div>35%</div><div>5%</div></div></div>
2	E	214	<div><div>%</div><div><div></div><div>71%</div><div>25%</div><div>•</div></div></div>
3	D	226	<div><div>11%</div><div><div></div><div>59%</div><div>33%</div><div>6%</div><div>•</div></div></div>
3	F	226	<div><div>4%</div><div><div></div><div>62%</div><div>31%</div><div>5%</div><div>•</div></div></div>

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Mol	Chain	Length	Quality of chain
4	G	2	 100%
4	H	2	 100%
4	I	2	 100%
4	K	2	 100%
5	J	3	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	G	1	X	-	-	-
4	NAG	G	2	-	-	-	X
4	NAG	H	2	-	-	-	X
4	NAG	I	1	X	-	-	-
4	NAG	I	2	-	-	-	X
5	NAG	J	2	-	-	-	X
5	BMA	J	3	-	-	-	X
6	NAG	A	1006	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 15481 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 Receptor protein-tyrosine kinase erbB-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4277	2656	769	805	47			
1	B	568	Total	C	N	O	S	0	0	0
			4381	2723	788	821	49			

- Molecule 2 is a protein called Pertuzumab Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	214	Total	C	N	O	S	0	0	0
			1657	1043	272	336	6			
2	E	214	Total	C	N	O	S	0	0	0
			1657	1043	272	336	6			

- Molecule 3 is a protein called Pertuzumab Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	222	Total	C	N	O	S	0	0	0
			1665	1051	280	327	7			
3	F	222	Total	C	N	O	S	0	0	0
			1665	1051	280	327	7			

- 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	G	2	Total	C	N	O		0	0	0
			28	16	2	10				

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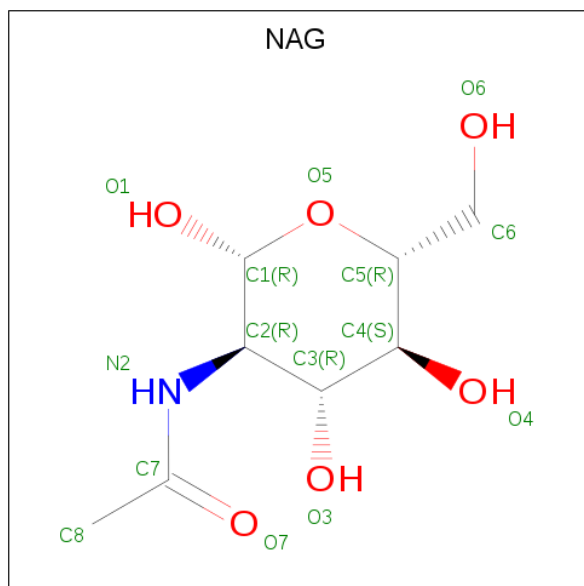
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 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
5	J	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

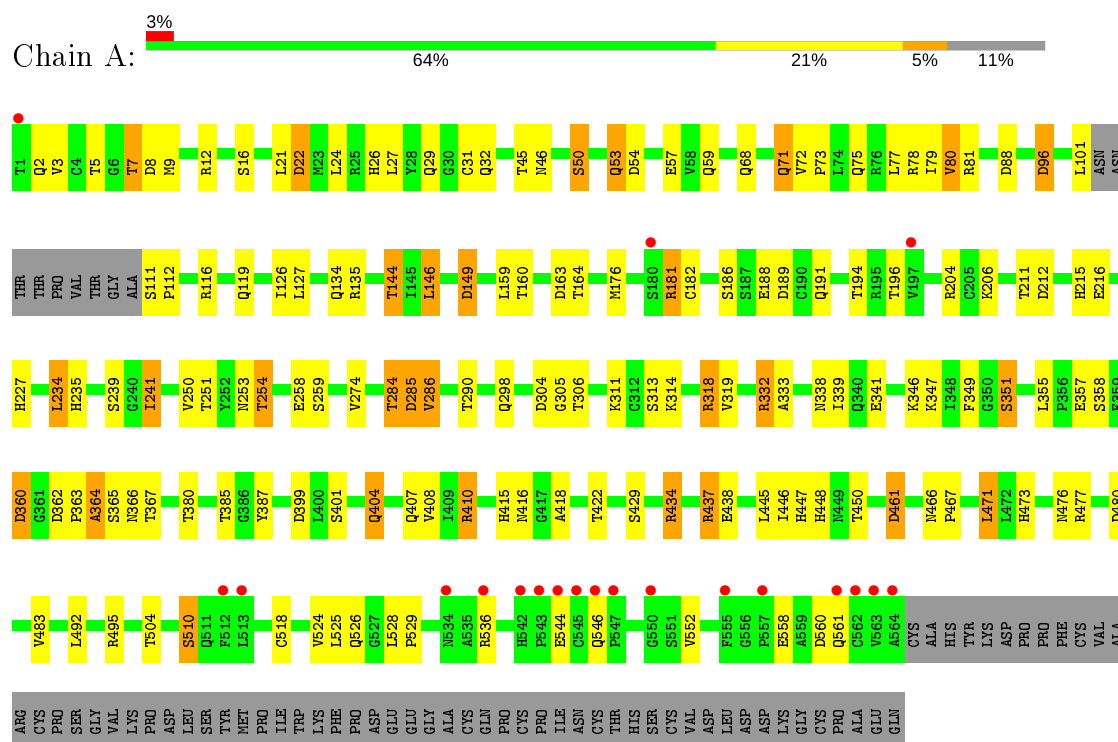


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

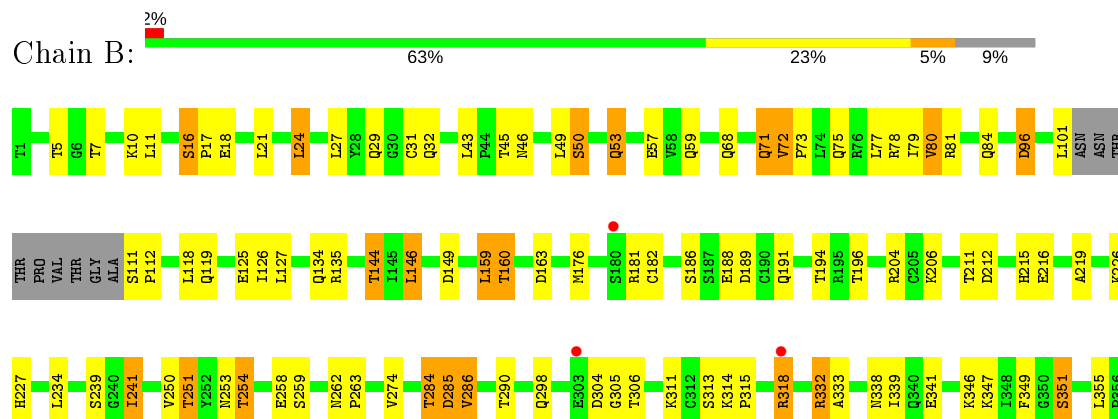
### 3 Residue-property plots

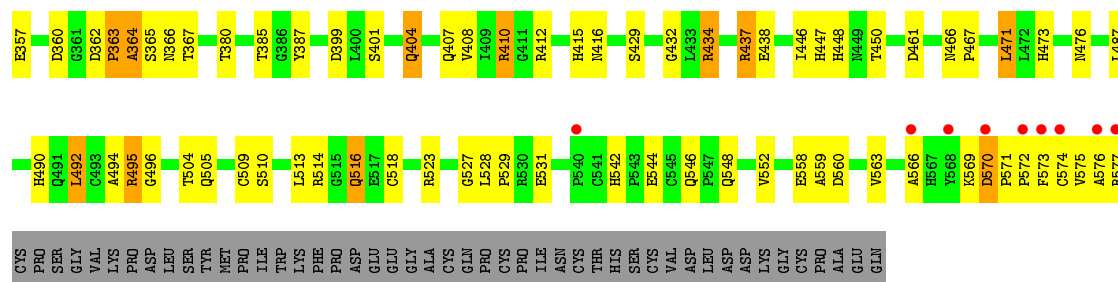
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Receptor protein-tyrosine kinase erbB-2

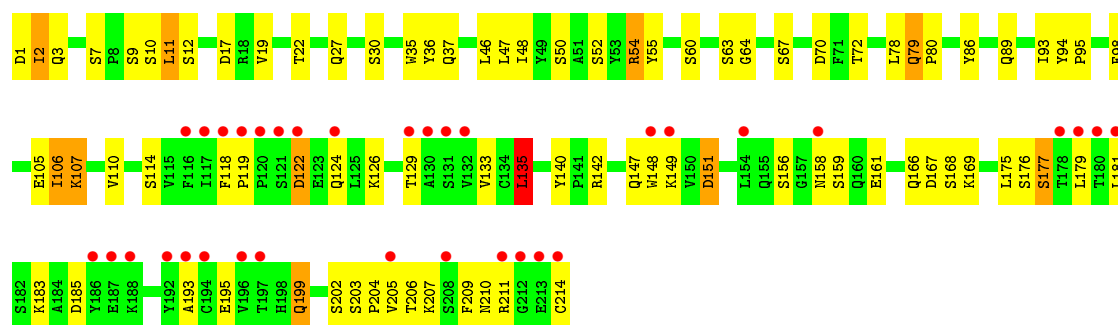


- Molecule 1: Receptor protein-tyrosine kinase erbB-2

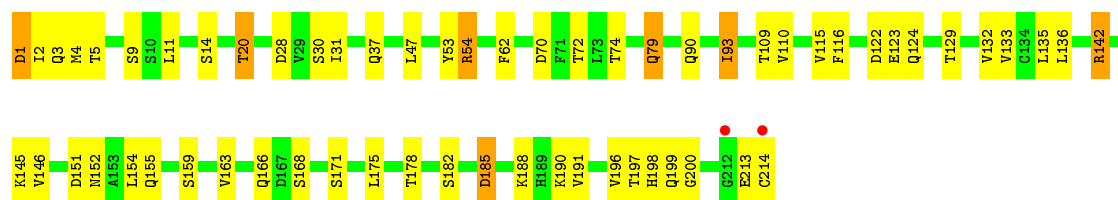




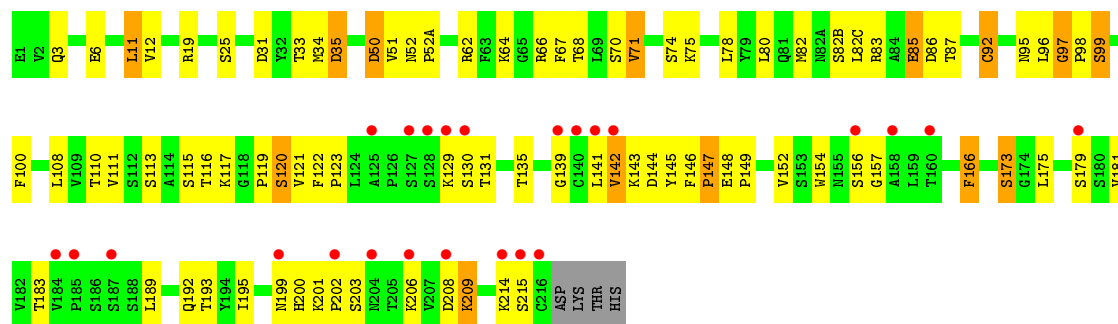
• Molecule 2: Pertuzumab Fab light chain



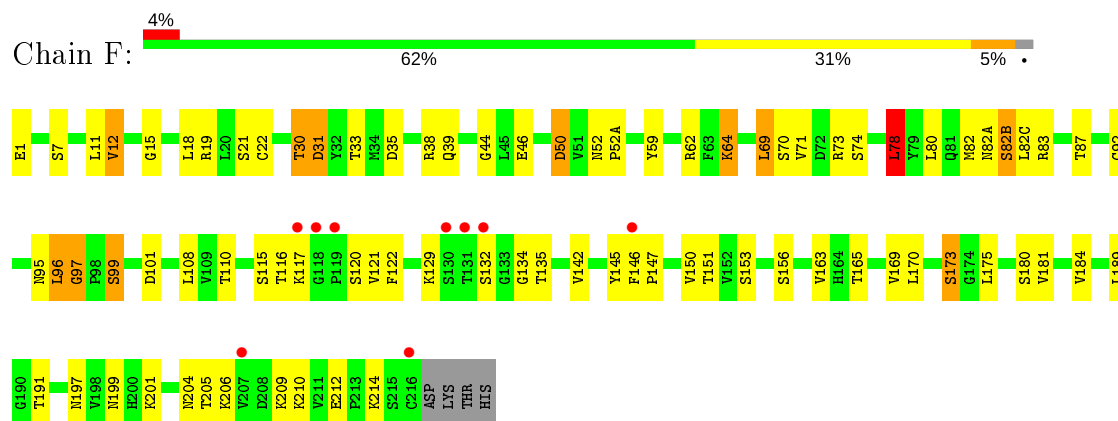
• Molecule 2: Pertuzumab Fab light chain



• Molecule 3: Pertuzumab Fab heavy chain



• Molecule 3: Pertuzumab Fab heavy chain



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

Chain G: 

MAG1  
MAG2

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

Chain H: 

MAG1  
MAG2

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

Chain I: 

MAG1  
MAG2

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

Chain K: 

MAG1  
MAG2

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

Chain J: 

MAG1  
MAG2  
BXI3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.41Å 139.41Å 356.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.25 29.85 – 3.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-3.25) 99.9 (29.85-3.25)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.11 (at 3.24Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.224 , 0.268 0.226 , 0.261	Depositor DCC
$R_{free}$ test set	2835 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	81.6	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 59.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	15481	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: BMA, 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	0.43	0/4374	0.77	15/5950 (0.3%)
1	B	0.44	0/4483	0.75	10/6099 (0.2%)
2	C	0.38	0/1695	0.71	6/2301 (0.3%)
2	E	0.39	0/1695	0.71	5/2301 (0.2%)
3	D	0.39	0/1706	0.72	5/2324 (0.2%)
3	F	0.42	0/1706	0.76	4/2324 (0.2%)
All	All	0.42	0/15659	0.75	45/21299 (0.2%)

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	ARG	NE-CZ-NH2	9.48	125.04	120.30
1	A	318	ARG	NE-CZ-NH1	-9.13	115.73	120.30
3	F	97	GLY	N-CA-C	-8.23	92.52	113.10
3	D	97	GLY	N-CA-C	-7.86	93.45	113.10
1	B	318	ARG	NE-CZ-NH2	-7.13	116.74	120.30
1	B	318	ARG	NE-CZ-NH1	6.86	123.73	120.30
2	E	185	ASP	CB-CG-OD2	6.36	124.02	118.30
3	F	31	ASP	CB-CG-OD2	6.34	124.01	118.30
1	A	212	ASP	CB-CG-OD2	6.34	124.00	118.30
1	B	96	ASP	CB-CG-OD2	6.32	123.99	118.30
3	D	50	ASP	CB-CG-OD2	6.24	123.91	118.30
1	B	212	ASP	CB-CG-OD2	6.19	123.87	118.30
3	D	35	ASP	CB-CG-OD2	6.01	123.71	118.30
3	F	78	LEU	CA-CB-CG	5.77	128.56	115.30
1	A	8	ASP	CB-CG-OD2	5.76	123.48	118.30
1	A	22	ASP	CB-CG-OD2	5.61	123.35	118.30
2	E	28	ASP	CB-CG-OD2	5.57	123.32	118.30
1	A	399	ASP	CB-CG-OD2	5.49	123.24	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	ASP	CB-CG-OD2	5.40	123.16	118.30
2	E	1	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	285	ASP	CB-CG-OD2	5.36	123.13	118.30
1	A	88	ASP	CB-CG-OD2	5.31	123.08	118.30
2	E	151	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	149	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	399	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	570	ASP	CB-CG-OD2	5.26	123.03	118.30
2	C	167	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	96	ASP	CB-CG-OD2	5.19	122.97	118.30
2	C	185	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	560	ASP	CB-CG-OD2	5.18	122.97	118.30
1	A	360	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	480	ASP	CB-CG-OD2	5.15	122.94	118.30
2	C	122	ASP	CB-CG-OD2	5.13	122.92	118.30
3	D	208	ASP	CB-CG-OD2	5.12	122.91	118.30
3	F	50	ASP	CB-CG-OD2	5.11	122.90	118.30
2	C	17	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	285	ASP	CB-CG-OD2	5.07	122.87	118.30
1	A	54	ASP	CB-CG-OD2	5.07	122.86	118.30
2	E	122	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	159	LEU	CA-CB-CG	5.06	126.94	115.30
2	C	151	ASP	CB-CG-OD2	5.06	122.86	118.30
2	C	70	ASP	CB-CG-OD2	5.04	122.83	118.30
3	D	144	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	304	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	560	ASP	CB-CG-OD2	5.01	122.81	118.30

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	4277	0	4103	60	0
1	B	4381	0	4198	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1657	0	1604	25	0
2	E	1657	0	1604	19	0
3	D	1665	0	1623	36	0
3	F	1665	0	1623	37	0
4	G	28	0	25	0	0
4	H	28	0	25	0	0
4	I	28	0	25	0	0
4	K	28	0	25	0	0
5	J	39	0	34	0	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
All	All	15481	0	14915	248	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 8.

All (248) 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:E:142:ARG:HG2	2:E:142:ARG:HH11	1.06	1.08
3:F:30:THR:HG21	3:F:73:ARG:NH2	1.76	1.00
3:F:30:THR:HG21	3:F:73:ARG:HH21	1.23	0.99
1:A:528:LEU:HB2	1:A:529:PRO:HD3	1.50	0.91
2:E:142:ARG:HG2	2:E:142:ARG:NH1	1.82	0.90
1:A:447:HIS:HD2	1:A:448:HIS:HD2	1.19	0.89
1:B:528:LEU:HB2	1:B:529:PRO:HD3	1.56	0.86
1:B:447:HIS:HD2	1:B:448:HIS:HD2	1.25	0.84
1:A:362:ASP:OD2	1:A:364:ALA:HB3	1.85	0.76
1:B:408:VAL:HG12	1:B:438:GLU:HB3	1.65	0.76
1:A:447:HIS:HD2	1:A:448:HIS:CD2	2.04	0.75
3:F:87:THR:HG23	3:F:110:THR:HA	1.67	0.74
3:D:34:MET:HB2	3:D:78:LEU:HD21	1.70	0.74
1:A:408:VAL:HG12	1:A:438:GLU:HB3	1.68	0.73
3:F:95:ASN:OD1	3:F:99:SER:O	2.06	0.73
1:B:447:HIS:HD2	1:B:448:HIS:CD2	2.05	0.73
1:A:50:SER:O	1:A:53:GLN:HG2	1.89	0.72
1:B:362:ASP:OD2	1:B:364:ALA:HB3	1.89	0.72
3:D:97:GLY:C	3:D:99:SER:H	1.93	0.72
1:B:50:SER:O	1:B:53:GLN:HG2	1.90	0.71
1:A:528:LEU:CB	1:A:529:PRO:HD3	2.18	0.71
1:A:447:HIS:CD2	1:A:448:HIS:HD2	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:30:THR:CG2	3:F:73:ARG:HH21	2.02	0.69
3:F:12:VAL:HG21	3:F:82(C):LEU:HD13	1.74	0.69
1:A:186:SER:HB3	1:A:189:ASP:OD1	1.93	0.69
1:B:347:LYS:HE2	1:B:349:PHE:CZ	2.29	0.68
2:E:142:ARG:CG	2:E:142:ARG:HH11	1.95	0.68
1:B:186:SER:HB3	1:B:189:ASP:OD1	1.94	0.67
2:E:136:LEU:HD11	2:E:196:VAL:HG21	1.75	0.67
2:C:37:GLN:HB2	2:C:47:LEU:HD11	1.76	0.67
1:A:338:ASN:O	1:A:341:GLU:HB2	1.95	0.67
1:A:144:THR:HG23	1:A:181:ARG:HA	1.76	0.66
1:B:338:ASN:O	1:B:341:GLU:HB2	1.95	0.66
1:A:227:HIS:CD2	1:A:241:ILE:HG23	2.31	0.66
1:B:144:THR:HG23	1:B:181:ARG:HA	1.79	0.65
1:B:415:HIS:CE1	1:B:416:ASN:ND2	2.65	0.64
1:A:347:LYS:HE2	1:A:349:PHE:CZ	2.34	0.63
3:F:69:LEU:HD22	3:F:80:LEU:HD13	1.82	0.62
1:A:332:ARG:CB	1:A:332:ARG:HH11	2.13	0.62
1:B:432:GLY:HA2	1:B:505:GLN:OE1	2.00	0.62
3:D:120:SER:HB2	3:D:122:PHE:CZ	2.34	0.62
2:C:35:TRP:HB2	2:C:48:ILE:HB	1.82	0.62
2:C:135:LEU:HD22	3:D:181:VAL:HG11	1.81	0.61
1:A:12:ARG:NH1	1:A:416:ASN:OD1	2.33	0.61
3:F:22:CYS:HB3	3:F:78:LEU:HD13	1.81	0.61
1:B:447:HIS:CD2	1:B:448:HIS:HD2	2.12	0.61
1:B:514:ARG:NH1	1:B:531:GLU:OE2	2.34	0.61
3:F:116:THR:HG22	3:F:147:PRO:HD3	1.82	0.61
1:A:57:GLU:HG3	1:A:79:ILE:HG23	1.81	0.61
2:C:94:TYR:CD2	2:C:95:PRO:HA	2.36	0.60
2:C:161:GLU:HG2	2:C:175:LEU:HD21	1.83	0.60
3:D:51:VAL:CG1	3:D:78:LEU:HD23	2.32	0.60
3:D:119:PRO:HB3	3:D:145:TYR:HB3	1.82	0.60
1:A:471:LEU:HD13	1:A:473:HIS:CD2	2.36	0.60
1:B:253:ASN:O	1:B:254:THR:HB	2.01	0.60
1:B:215:HIS:CD2	1:B:227:HIS:HB3	2.37	0.59
3:D:12:VAL:HG21	3:D:82(C):LEU:HD13	1.83	0.59
1:B:471:LEU:HD13	1:B:473:HIS:CD2	2.37	0.59
1:B:81:ARG:HG2	1:B:127:LEU:HD12	1.84	0.59
1:A:332:ARG:HB2	1:A:332:ARG:HH11	1.67	0.59
1:A:81:ARG:HG2	1:A:127:LEU:HD12	1.85	0.59
1:B:227:HIS:CD2	1:B:241:ILE:HG23	2.38	0.58
1:A:71:GLN:HE22	1:A:75:GLN:HE22	1.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:SER:HB3	1:A:387:TYR:H	1.68	0.58
1:A:528:LEU:HB2	1:A:529:PRO:CD	2.29	0.58
3:F:33:THR:HG22	3:F:52:ASN:HA	1.84	0.58
1:A:253:ASN:O	1:A:254:THR:HB	2.03	0.57
1:A:415:HIS:CE1	1:A:416:ASN:ND2	2.73	0.56
1:B:332:ARG:HH11	1:B:332:ARG:CB	2.18	0.56
3:F:52(A):PRO:HA	3:F:71:VAL:HG21	1.87	0.56
3:D:97:GLY:C	3:D:99:SER:N	2.59	0.56
3:F:97:GLY:C	3:F:99:SER:H	2.09	0.56
1:B:57:GLU:HG3	1:B:79:ILE:HG23	1.88	0.56
1:A:144:THR:CG2	1:A:182:CYS:H	2.17	0.56
3:F:59:TYR:CE1	3:F:64:LYS:HB2	2.41	0.56
1:B:290:THR:HG21	3:F:31:ASP:OD2	2.06	0.56
2:C:149:LYS:HD3	2:C:195:GLU:HG3	1.87	0.55
3:F:35:ASP:OD2	3:F:50:ASP:HB2	2.07	0.54
2:C:79:GLN:HG3	2:C:80:PRO:HD2	1.89	0.54
1:A:194:THR:HG22	1:A:204:ARG:HD3	1.89	0.54
2:C:11:LEU:HD21	2:C:19:VAL:HG13	1.89	0.54
1:B:73:PRO:HA	1:B:75:GLN:HE22	1.73	0.54
1:A:492:LEU:O	1:A:510:SER:HB3	2.07	0.54
3:F:38:ARG:NE	3:F:46:GLU:OE1	2.41	0.54
1:A:446:ILE:HD12	1:A:471:LEU:HD21	1.90	0.54
2:E:37:GLN:HB2	2:E:47:LEU:HD11	1.89	0.54
2:C:79:GLN:HA	2:C:79:GLN:HE21	1.73	0.53
1:B:144:THR:CG2	1:B:182:CYS:H	2.21	0.53
3:D:119:PRO:HB2	3:D:142:VAL:HG12	1.90	0.53
1:A:215:HIS:CD2	1:A:227:HIS:HB3	2.44	0.53
1:B:71:GLN:HE22	1:B:75:GLN:HE22	1.56	0.53
2:C:46:LEU:HD23	2:C:55:TYR:CD1	2.44	0.53
2:C:148:TRP:HE1	2:C:177:SER:HB3	1.73	0.53
2:E:54:ARG:HD3	2:E:62:PHE:O	2.09	0.52
3:D:173:SER:HB2	3:D:175:LEU:HD12	1.92	0.52
1:A:290:THR:HG21	3:D:31:ASP:OD2	2.10	0.52
1:A:404:GLN:HG2	1:A:434:ARG:NH1	2.25	0.52
3:D:166:PHE:HB2	3:D:179:SER:O	2.09	0.52
1:B:351:SER:HB3	1:B:387:TYR:H	1.75	0.51
3:F:165:THR:HG23	3:F:180:SER:HB2	1.92	0.51
1:B:385:THR:HA	1:B:410:ARG:HB2	1.93	0.50
1:B:71:GLN:CD	1:B:119:GLN:HE21	2.15	0.50
3:D:123:PRO:HD3	3:D:209:LYS:HG2	1.93	0.50
1:A:7:THR:HG22	1:A:418:ALA:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:66:ARG:NH1	3:D:86:ASP:OD2	2.44	0.50
2:E:136:LEU:HD11	2:E:196:VAL:CG2	2.41	0.50
1:A:333:ALA:HB2	1:A:355:LEU:HD22	1.94	0.50
1:B:404:GLN:HG2	1:B:434:ARG:NH1	2.26	0.50
1:B:490:HIS:CE1	1:B:492:LEU:HD22	2.46	0.50
3:F:39:GLN:HG3	3:F:44:GLY:O	2.12	0.50
1:B:286:VAL:HG22	3:F:33:THR:HG23	1.94	0.50
1:A:466:ASN:HB2	1:A:467:PRO:HD2	1.94	0.49
2:E:135:LEU:CD1	3:F:181:VAL:HG21	2.42	0.49
1:A:528:LEU:CB	1:A:529:PRO:CD	2.89	0.49
1:B:523:ARG:HG2	1:B:527:GLY:HA3	1.93	0.49
1:B:401:SER:O	1:B:404:GLN:HB2	2.12	0.49
2:E:146:VAL:HG21	2:E:175:LEU:HD22	1.95	0.49
1:B:466:ASN:HB2	1:B:467:PRO:HD2	1.95	0.49
3:D:97:GLY:O	3:D:99:SER:N	2.46	0.49
1:B:446:ILE:HD12	1:B:471:LEU:HD21	1.95	0.48
3:F:120:SER:HB3	3:F:122:PHE:CZ	2.48	0.48
1:B:528:LEU:HB2	1:B:529:PRO:CD	2.38	0.48
3:D:200:HIS:HB3	3:D:203:SER:HB3	1.96	0.48
1:A:284:THR:CG2	1:A:286:VAL:H	2.26	0.48
1:A:73:PRO:HA	1:A:75:GLN:HE22	1.79	0.48
1:B:446:ILE:HG22	1:B:476:ASN:HD21	1.77	0.48
1:B:286:VAL:CG2	3:F:33:THR:HG23	2.44	0.48
3:D:200:HIS:CE1	3:D:202:PRO:HD2	2.49	0.48
1:A:446:ILE:HG22	1:A:476:ASN:HD21	1.78	0.48
1:B:284:THR:CG2	1:B:286:VAL:H	2.27	0.48
3:F:146:PHE:HB2	3:F:175:LEU:HD23	1.96	0.47
1:B:332:ARG:HH11	1:B:332:ARG:HB2	1.79	0.47
1:A:251:THR:O	1:A:259:SER:HA	2.14	0.47
3:F:97:GLY:C	3:F:99:SER:N	2.67	0.47
2:C:54:ARG:NH1	2:C:60:SER:HA	2.28	0.47
1:A:385:THR:HA	1:A:410:ARG:HB2	1.96	0.47
3:F:173:SER:HB2	3:F:175:LEU:HD12	1.96	0.47
1:A:401:SER:O	1:A:404:GLN:HB2	2.14	0.47
2:E:133:VAL:HG22	2:E:178:THR:HG23	1.97	0.47
3:D:139:GLY:HA2	3:D:154:TRP:CZ2	2.49	0.47
2:E:198:HIS:CD2	2:E:200:GLY:H	2.32	0.47
3:F:71:VAL:HG12	3:F:78:LEU:HB3	1.97	0.47
2:E:136:LEU:HB2	2:E:175:LEU:HB3	1.97	0.47
1:A:285:ASP:OD2	1:A:311:LYS:HE2	2.15	0.47
3:D:35:ASP:OD1	3:D:50:ASP:OD1	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:PRO:HA	1:B:572:PRO:HA	1.71	0.46
3:D:11:LEU:HD13	3:D:146:PHE:HE1	1.81	0.46
1:A:96:ASP:HA	1:A:135:ARG:O	2.15	0.46
1:B:251:THR:O	1:B:259:SER:HA	2.15	0.46
2:C:175:LEU:HD23	2:C:176:SER:N	2.29	0.46
3:D:12:VAL:HG23	3:D:111:VAL:HG22	1.96	0.46
3:D:87:THR:HG23	3:D:110:THR:HA	1.98	0.46
1:B:96:ASP:HA	1:B:135:ARG:O	2.15	0.46
1:B:333:ALA:HB2	1:B:355:LEU:HD22	1.98	0.46
3:D:52(A):PRO:HA	3:D:71:VAL:HG21	1.97	0.46
1:A:2:GLN:HG3	1:A:3:VAL:HG23	1.98	0.46
1:B:407:GLN:HB3	1:B:437:ARG:HE	1.80	0.46
1:B:516:GLN:HE21	1:B:516:GLN:HA	1.82	0.45
2:E:4:MET:HE2	2:E:90:GLN:HB3	1.97	0.45
1:A:22:ASP:O	1:A:26:HIS:HD2	1.99	0.45
1:B:118:LEU:HA	1:B:118:LEU:HD23	1.89	0.45
2:C:118:PHE:HA	2:C:119:PRO:HD3	1.84	0.45
2:E:20:THR:HG23	2:E:74:THR:HG23	1.97	0.45
1:A:284:THR:HG23	1:A:286:VAL:H	1.82	0.45
2:C:19:VAL:HG21	2:C:78:LEU:HD22	1.99	0.45
1:A:164:THR:OG1	1:B:160:THR:HB	2.16	0.45
1:B:415:HIS:CE1	1:B:416:ASN:HD22	2.35	0.45
1:B:290:THR:HG21	3:F:31:ASP:OD1	2.17	0.45
1:A:351:SER:HB3	1:A:387:TYR:O	2.16	0.45
3:F:96:LEU:HD22	3:F:101:ASP:HB3	1.98	0.45
3:D:35:ASP:OD1	3:D:95:ASN:HB2	2.15	0.45
1:B:10:LYS:HB3	1:B:11:LEU:H	1.61	0.45
1:B:492:LEU:HD23	1:B:518:CYS:O	2.17	0.44
2:E:116:PHE:HB2	2:E:135:LEU:HB3	2.00	0.44
3:F:146:PHE:HA	3:F:147:PRO:HA	1.73	0.44
2:C:2:ILE:H	2:C:2:ILE:HG12	1.67	0.44
3:D:148:GLU:HA	3:D:149:PRO:HA	1.66	0.44
3:D:201:LYS:HB2	3:D:202:PRO:HD3	1.99	0.44
2:E:135:LEU:HD11	3:F:181:VAL:HG21	2.00	0.44
1:B:559:ALA:HB1	1:B:574:CYS:H	1.83	0.44
2:C:36:TYR:HE2	2:C:89:GLN:OE1	2.01	0.44
1:A:355:LEU:O	1:A:358:SER:HB2	2.18	0.44
1:B:80:VAL:HG13	1:B:126:ILE:HG12	1.99	0.44
3:F:96:LEU:HD12	3:F:96:LEU:HA	1.75	0.44
3:F:15:GLY:HA2	3:F:82(B):SER:HA	2.00	0.44
1:B:490:HIS:HE1	1:B:492:LEU:HD22	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:ASP:HA	1:B:571:PRO:HD3	1.90	0.43
3:D:119:PRO:CB	3:D:145:TYR:HB3	2.47	0.43
1:B:548:GLN:HG3	1:B:563:VAL:HG11	1.99	0.43
3:F:145:TYR:CE2	3:F:150:VAL:HG13	2.54	0.43
1:B:487:LEU:HA	1:B:487:LEU:HD23	1.91	0.43
2:C:193:ALA:HB1	2:C:206:THR:CG2	2.49	0.43
3:D:52:ASN:HA	3:D:52(A):PRO:HD3	1.83	0.43
1:A:422:THR:HA	1:A:445:LEU:O	2.19	0.43
1:B:194:THR:HG22	1:B:204:ARG:HD3	2.01	0.43
3:D:146:PHE:HA	3:D:147:PRO:HA	1.70	0.43
3:D:3:GLN:HG3	3:D:25:SER:OG	2.19	0.42
1:A:80:VAL:HG13	1:A:126:ILE:HG12	2.01	0.42
2:C:106:ILE:HG23	2:C:166:GLN:HE21	1.83	0.42
1:B:315:PRO:HD3	2:E:53:TYR:CE1	2.54	0.42
1:A:407:GLN:HB3	1:A:437:ARG:HE	1.84	0.42
1:B:494:ALA:C	1:B:496:GLY:N	2.72	0.42
3:F:121:VAL:HG22	3:F:142:VAL:HG13	2.00	0.42
1:A:9:MET:O	1:A:12:ARG:HB2	2.20	0.42
2:C:52:SER:HA	2:C:64:GLY:O	2.20	0.42
1:A:146:LEU:HD11	1:A:196:THR:HG21	2.01	0.42
1:B:125:GLU:OE1	1:B:219:ALA:O	2.38	0.42
3:D:200:HIS:ND1	3:D:202:PRO:HD2	2.35	0.42
3:D:85:GLU:H	3:D:85:GLU:HG3	1.69	0.42
2:E:93:ILE:HD13	2:E:93:ILE:HA	1.87	0.42
3:F:69:LEU:CD2	3:F:80:LEU:HD13	2.48	0.42
1:B:351:SER:HB3	1:B:387:TYR:O	2.19	0.42
2:C:107:LYS:HA	2:C:140:TYR:OH	2.19	0.42
3:D:67:PHE:HB3	3:D:80:LEU:HD11	2.02	0.42
3:D:95:ASN:OD1	3:D:98:PRO:HA	2.20	0.41
2:E:79:GLN:NE2	2:E:79:GLN:HA	2.35	0.41
1:A:111:SER:N	1:A:112:PRO:HD2	2.36	0.41
1:A:134:GLN:HA	1:A:163:ASP:HB3	2.02	0.41
1:B:111:SER:N	1:B:112:PRO:HD2	2.35	0.41
1:B:146:LEU:HD12	1:B:149:ASP:HB2	2.01	0.41
1:B:410:ARG:HD3	1:B:412:ARG:NH2	2.34	0.41
2:C:79:GLN:HA	2:C:79:GLN:NE2	2.36	0.41
1:B:17:PRO:HD2	1:B:18:GLU:OE1	2.21	0.41
1:B:16:SER:HA	1:B:17:PRO:HD3	1.89	0.41
3:F:97:GLY:O	3:F:99:SER:N	2.54	0.41
1:B:146:LEU:HD11	1:B:196:THR:HG21	2.02	0.41
2:C:203:SER:HA	2:C:204:PRO:HD2	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:37:GLN:HG3	2:C:86:TYR:CE2	2.55	0.41
1:A:146:LEU:HD12	1:A:149:ASP:HB2	2.02	0.41
1:A:234:LEU:HD13	1:A:235:HIS:CE1	2.56	0.41
1:B:134:GLN:HA	1:B:163:ASP:HB3	2.02	0.41
1:B:284:THR:HG23	1:B:286:VAL:H	1.86	0.41
3:D:6:GLU:HG3	3:D:92:CYS:HB3	2.03	0.41
3:D:35:ASP:OD2	3:D:50:ASP:HB2	2.21	0.41
1:A:319:VAL:HG13	1:A:349:PHE:CD1	2.56	0.41
1:B:559:ALA:HB3	1:B:573:PHE:HD2	1.85	0.41
1:A:71:GLN:CD	1:A:119:GLN:HE21	2.24	0.41
1:B:43:LEU:HD13	1:B:49:LEU:HD21	2.03	0.41
1:B:542:HIS:HD2	1:B:544:GLU:HB2	1.86	0.41
1:B:72:VAL:HA	1:B:73:PRO:HD3	1.91	0.41
1:B:262:ASN:HA	1:B:263:PRO:HD2	1.91	0.40
1:B:548:GLN:HG3	1:B:563:VAL:CG1	2.52	0.40
2:C:89:GLN:HB2	2:C:98:PHE:CD2	2.55	0.40
1:B:24:LEU:HD23	1:B:43:LEU:HD21	2.03	0.40
1:B:285:ASP:OD2	1:B:311:LYS:HE2	2.21	0.40
1:B:362:ASP:HA	1:B:363:PRO:HD2	1.93	0.40
3:F:59:TYR:HE1	3:F:64:LYS:HB2	1.84	0.40
1:B:546:GLN:HB2	1:B:566:ALA:HA	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	551/624 (88%)	503 (91%)	41 (7%)	7 (1%)	12	41
1	B	564/624 (90%)	513 (91%)	43 (8%)	8 (1%)	11	40
2	C	212/214 (99%)	185 (87%)	23 (11%)	4 (2%)	8	34
2	E	212/214 (99%)	192 (91%)	18 (8%)	2 (1%)	17	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	220/226 (97%)	195 (89%)	22 (10%)	3 (1%)	11	40
3	F	220/226 (97%)	197 (90%)	19 (9%)	4 (2%)	8	35
All	All	1979/2128 (93%)	1785 (90%)	166 (8%)	28 (1%)	11	40

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	364	ALA
1	A	366	ASN
1	A	404	GLN
1	B	364	ALA
1	B	366	ASN
1	B	404	GLN
1	B	576	ALA
2	E	152	ASN
1	A	363	PRO
1	B	363	PRO
2	C	30	SER
2	E	30	SER
1	A	461	ASP
1	B	313	SER
1	B	495	ARG
2	C	151	ASP
1	A	313	SER
2	C	135	LEU
3	F	96	LEU
3	F	134	GLY
3	F	156	SER
3	D	96	LEU
3	F	18	LEU
2	C	199	GLN
1	A	305	GLY
1	B	305	GLY
3	D	157	GLY
3	D	147	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	478/538 (89%)	401 (84%)	77 (16%)	2	10
1	B	489/538 (91%)	414 (85%)	75 (15%)	2	12
2	C	188/188 (100%)	141 (75%)	47 (25%)	0	2
2	E	188/188 (100%)	149 (79%)	39 (21%)	1	4
3	D	187/191 (98%)	142 (76%)	45 (24%)	0	2
3	F	187/191 (98%)	143 (76%)	44 (24%)	1	3
All	All	1717/1834 (94%)	1390 (81%)	327 (19%)	1	6

All (327) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	7	THR
1	A	16	SER
1	A	21	LEU
1	A	24	LEU
1	A	27	LEU
1	A	29	GLN
1	A	31	CYS
1	A	32	GLN
1	A	45	THR
1	A	46	ASN
1	A	50	SER
1	A	53	GLN
1	A	59	GLN
1	A	68	GLN
1	A	71	GLN
1	A	72	VAL
1	A	77	LEU
1	A	78	ARG
1	A	80	VAL
1	A	101	LEU
1	A	116	ARG
1	A	144	THR
1	A	146	LEU
1	A	159	LEU
1	A	160	THR
1	A	176	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	181	ARG
1	A	188	GLU
1	A	191	GLN
1	A	206	LYS
1	A	211	THR
1	A	216	GLU
1	A	234	LEU
1	A	239	SER
1	A	241	ILE
1	A	250	VAL
1	A	254	THR
1	A	258	GLU
1	A	274	VAL
1	A	284	THR
1	A	286	VAL
1	A	298	GLN
1	A	306	THR
1	A	314	LYS
1	A	318	ARG
1	A	332	ARG
1	A	339	ILE
1	A	346	LYS
1	A	351	SER
1	A	357	GLU
1	A	360	ASP
1	A	365	SER
1	A	367	THR
1	A	380	THR
1	A	410	ARG
1	A	429	SER
1	A	434	ARG
1	A	437	ARG
1	A	450	THR
1	A	461	ASP
1	A	471	LEU
1	A	477	ARG
1	A	483	VAL
1	A	495	ARG
1	A	504	THR
1	A	510	SER
1	A	518	CYS
1	A	524	VAL

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Mol	Chain	Res	Type
1	A	525	LEU
1	A	526	GLN
1	A	536	ARG
1	A	544	GLU
1	A	546	GLN
1	A	552	VAL
1	A	558	GLU
1	A	561	GLN
1	B	5	THR
1	B	7	THR
1	B	16	SER
1	B	21	LEU
1	B	24	LEU
1	B	27	LEU
1	B	29	GLN
1	B	31	CYS
1	B	32	GLN
1	B	45	THR
1	B	46	ASN
1	B	50	SER
1	B	53	GLN
1	B	59	GLN
1	B	68	GLN
1	B	71	GLN
1	B	72	VAL
1	B	77	LEU
1	B	78	ARG
1	B	80	VAL
1	B	84	GLN
1	B	101	LEU
1	B	144	THR
1	B	146	LEU
1	B	159	LEU
1	B	160	THR
1	B	176	MET
1	B	188	GLU
1	B	191	GLN
1	B	206	LYS
1	B	211	THR
1	B	216	GLU
1	B	226	LYS
1	B	234	LEU

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Mol	Chain	Res	Type
1	B	239	SER
1	B	241	ILE
1	B	250	VAL
1	B	251	THR
1	B	254	THR
1	B	258	GLU
1	B	274	VAL
1	B	284	THR
1	B	286	VAL
1	B	298	GLN
1	B	306	THR
1	B	314	LYS
1	B	318	ARG
1	B	332	ARG
1	B	339	ILE
1	B	346	LYS
1	B	351	SER
1	B	357	GLU
1	B	360	ASP
1	B	365	SER
1	B	367	THR
1	B	380	THR
1	B	410	ARG
1	B	429	SER
1	B	434	ARG
1	B	437	ARG
1	B	450	THR
1	B	461	ASP
1	B	471	LEU
1	B	492	LEU
1	B	495	ARG
1	B	504	THR
1	B	509	CYS
1	B	510	SER
1	B	513	LEU
1	B	516	GLN
1	B	552	VAL
1	B	558	GLU
1	B	569	LYS
1	B	575	VAL
1	B	577	ARG
2	C	1	ASP

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Mol	Chain	Res	Type
2	C	2	ILE
2	C	3	GLN
2	C	7	SER
2	C	9	SER
2	C	10	SER
2	C	11	LEU
2	C	12	SER
2	C	22	THR
2	C	27	GLN
2	C	50	SER
2	C	54	ARG
2	C	63	SER
2	C	67	SER
2	C	72	THR
2	C	79	GLN
2	C	93	ILE
2	C	105	GLU
2	C	106	ILE
2	C	107	LYS
2	C	110	VAL
2	C	114	SER
2	C	122	ASP
2	C	124	GLN
2	C	126	LYS
2	C	129	THR
2	C	133	VAL
2	C	135	LEU
2	C	142	ARG
2	C	147	GLN
2	C	156	SER
2	C	158	ASN
2	C	159	SER
2	C	168	SER
2	C	169	LYS
2	C	177	SER
2	C	179	LEU
2	C	181	LEU
2	C	183	LYS
2	C	199	GLN
2	C	202	SER
2	C	205	VAL
2	C	207	LYS

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Mol	Chain	Res	Type
2	C	209	PHE
2	C	210	ASN
2	C	211	ARG
2	C	214	CYS
3	D	11	LEU
3	D	19	ARG
3	D	33	THR
3	D	62	ARG
3	D	64	LYS
3	D	68	THR
3	D	70	SER
3	D	71	VAL
3	D	74	SER
3	D	75	LYS
3	D	82	MET
3	D	82(B)	SER
3	D	83	ARG
3	D	85	GLU
3	D	92	CYS
3	D	99	SER
3	D	100	PHE
3	D	108	LEU
3	D	113	SER
3	D	115	SER
3	D	116	THR
3	D	117	LYS
3	D	120	SER
3	D	121	VAL
3	D	129	LYS
3	D	130	SER
3	D	131	THR
3	D	135	THR
3	D	141	LEU
3	D	142	VAL
3	D	143	LYS
3	D	152	VAL
3	D	156	SER
3	D	166	PHE
3	D	173	SER
3	D	183	THR
3	D	189	LEU
3	D	192	GLN

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Mol	Chain	Res	Type
3	D	193	THR
3	D	195	ILE
3	D	199	ASN
3	D	206	LYS
3	D	209	LYS
3	D	214	LYS
3	D	215	SER
2	E	1	ASP
2	E	2	ILE
2	E	3	GLN
2	E	5	THR
2	E	9	SER
2	E	11	LEU
2	E	14	SER
2	E	20	THR
2	E	31	ILE
2	E	54	ARG
2	E	70	ASP
2	E	72	THR
2	E	79	GLN
2	E	93	ILE
2	E	109	THR
2	E	110	VAL
2	E	115	VAL
2	E	123	GLU
2	E	124	GLN
2	E	129	THR
2	E	132	VAL
2	E	142	ARG
2	E	145	LYS
2	E	154	LEU
2	E	155	GLN
2	E	159	SER
2	E	163	VAL
2	E	166	GLN
2	E	168	SER
2	E	171	SER
2	E	182	SER
2	E	185	ASP
2	E	188	LYS
2	E	190	LYS
2	E	191	VAL

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Mol	Chain	Res	Type
2	E	197	THR
2	E	199	GLN
2	E	213	GLU
2	E	214	CYS
3	F	1	GLU
3	F	7	SER
3	F	11	LEU
3	F	12	VAL
3	F	19	ARG
3	F	21	SER
3	F	30	THR
3	F	62	ARG
3	F	64	LYS
3	F	69	LEU
3	F	70	SER
3	F	74	SER
3	F	78	LEU
3	F	82	MET
3	F	82(A)	ASN
3	F	82(B)	SER
3	F	83	ARG
3	F	92	CYS
3	F	99	SER
3	F	108	LEU
3	F	115	SER
3	F	117	LYS
3	F	129	LYS
3	F	132	SER
3	F	135	THR
3	F	151	THR
3	F	153	SER
3	F	163	VAL
3	F	169	VAL
3	F	170	LEU
3	F	173	SER
3	F	184	VAL
3	F	189	LEU
3	F	191	THR
3	F	197	ASN
3	F	199	ASN
3	F	201	LYS
3	F	204	ASN

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Mol	Chain	Res	Type
3	F	205	THR
3	F	206	LYS
3	F	209	LYS
3	F	210	LYS
3	F	212	GLU
3	F	214	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	71	GLN
1	A	75	GLN
1	A	119	GLN
1	A	138	GLN
1	A	156	GLN
1	A	245	HIS
1	A	366	ASN
1	A	415	HIS
1	A	424	GLN
1	A	447	HIS
1	A	448	HIS
1	A	473	HIS
1	A	516	GLN
1	B	26	HIS
1	B	75	GLN
1	B	119	GLN
1	B	138	GLN
1	B	156	GLN
1	B	245	HIS
1	B	366	ASN
1	B	415	HIS
1	B	416	ASN
1	B	447	HIS
1	B	448	HIS
1	B	473	HIS
1	B	497	HIS
1	B	516	GLN
1	B	537	HIS
1	B	542	HIS
1	B	546	GLN
2	C	3	GLN

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Mol	Chain	Res	Type
2	C	79	GLN
2	C	147	GLN
2	C	160	GLN
2	C	166	GLN
3	D	76	ASN
2	E	79	GLN
2	E	155	GLN
2	E	198	HIS
2	E	210	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 ⓘ

11 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	G	1	1,4	14,14,15	1.29	1 (7%)	17,19,21	2.50	5 (29%)
4	NAG	G	2	4	14,14,15	0.76	0	17,19,21	1.47	1 (5%)
4	NAG	H	1	1,4	14,14,15	0.66	0	17,19,21	1.06	1 (5%)
4	NAG	H	2	4	14,14,15	0.58	0	17,19,21	1.52	3 (17%)
4	NAG	I	1	1,4	14,14,15	1.18	1 (7%)	17,19,21	2.34	5 (29%)
4	NAG	I	2	4	14,14,15	0.70	0	17,19,21	1.36	2 (11%)
5	NAG	J	1	1,5	14,14,15	0.62	0	17,19,21	1.12	1 (5%)
5	NAG	J	2	5	14,14,15	0.68	0	17,19,21	1.40	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BMA	J	3	5	11,11,12	0.61	0	15,15,17	1.26	1 (6%)
4	NAG	K	1	1,4	14,14,15	0.53	0	17,19,21	1.57	2 (11%)
4	NAG	K	2	4	14,14,15	0.51	0	17,19,21	0.84	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1	1,4	1/1/5/7	3/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	NAG	I	1	1,4	1/1/5/7	3/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
5	NAG	J	1	1,5	-	6/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
5	BMA	J	3	5	-	1/2/19/22	0/1/1/1
4	NAG	K	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1	NAG	C1-C2	2.62	1.56	1.52
4	I	1	NAG	C1-C2	2.46	1.56	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	NAG	C2-N2-C7	6.13	131.63	122.90
4	I	1	NAG	C2-N2-C7	5.77	131.12	122.90
4	K	1	NAG	C1-O5-C5	4.68	118.53	112.19
4	G	1	NAG	O4-C4-C3	4.40	120.53	110.35
4	H	2	NAG	C4-C3-C2	4.33	117.37	111.02
4	G	2	NAG	C1-O5-C5	4.07	117.70	112.19
4	I	1	NAG	O4-C4-C3	4.06	119.74	110.35
5	J	2	NAG	C4-C3-C2	4.00	116.88	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	3	BMA	O5-C5-C6	3.81	113.18	107.20
4	G	1	NAG	C3-C4-C5	-3.61	103.80	110.24
4	I	2	NAG	C1-O5-C5	3.45	116.86	112.19
4	I	1	NAG	C3-C4-C5	-3.19	104.55	110.24
5	J	1	NAG	C2-N2-C7	2.89	127.02	122.90
4	G	1	NAG	O5-C5-C4	-2.85	103.90	110.83
5	J	2	NAG	C3-C4-C5	2.83	115.29	110.24
4	K	1	NAG	O5-C5-C6	2.77	111.54	107.20
4	I	1	NAG	O5-C5-C4	-2.65	104.38	110.83
4	G	1	NAG	O5-C5-C6	2.60	111.28	107.20
4	H	2	NAG	C3-C4-C5	2.42	114.56	110.24
4	I	1	NAG	O5-C5-C6	2.37	110.92	107.20
4	H	1	NAG	C1-O5-C5	2.37	115.40	112.19
4	H	2	NAG	O5-C5-C6	2.23	110.70	107.20
4	I	2	NAG	O7-C7-N2	2.19	125.98	121.95
4	K	2	NAG	O5-C5-C6	2.19	110.63	107.20

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	G	1	NAG	C1
4	I	1	NAG	C1

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	K	2	NAG	C8-C7-N2-C2
4	K	2	NAG	O7-C7-N2-C2
4	G	1	NAG	C3-C2-N2-C7
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	I	1	NAG	C3-C2-N2-C7
4	I	1	NAG	C8-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2
4	K	1	NAG	C8-C7-N2-C2
4	K	1	NAG	O7-C7-N2-C2
5	J	2	NAG	C8-C7-N2-C2
5	J	2	NAG	O7-C7-N2-C2
4	H	2	NAG	C8-C7-N2-C2
4	H	2	NAG	O7-C7-N2-C2
5	J	1	NAG	C4-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6

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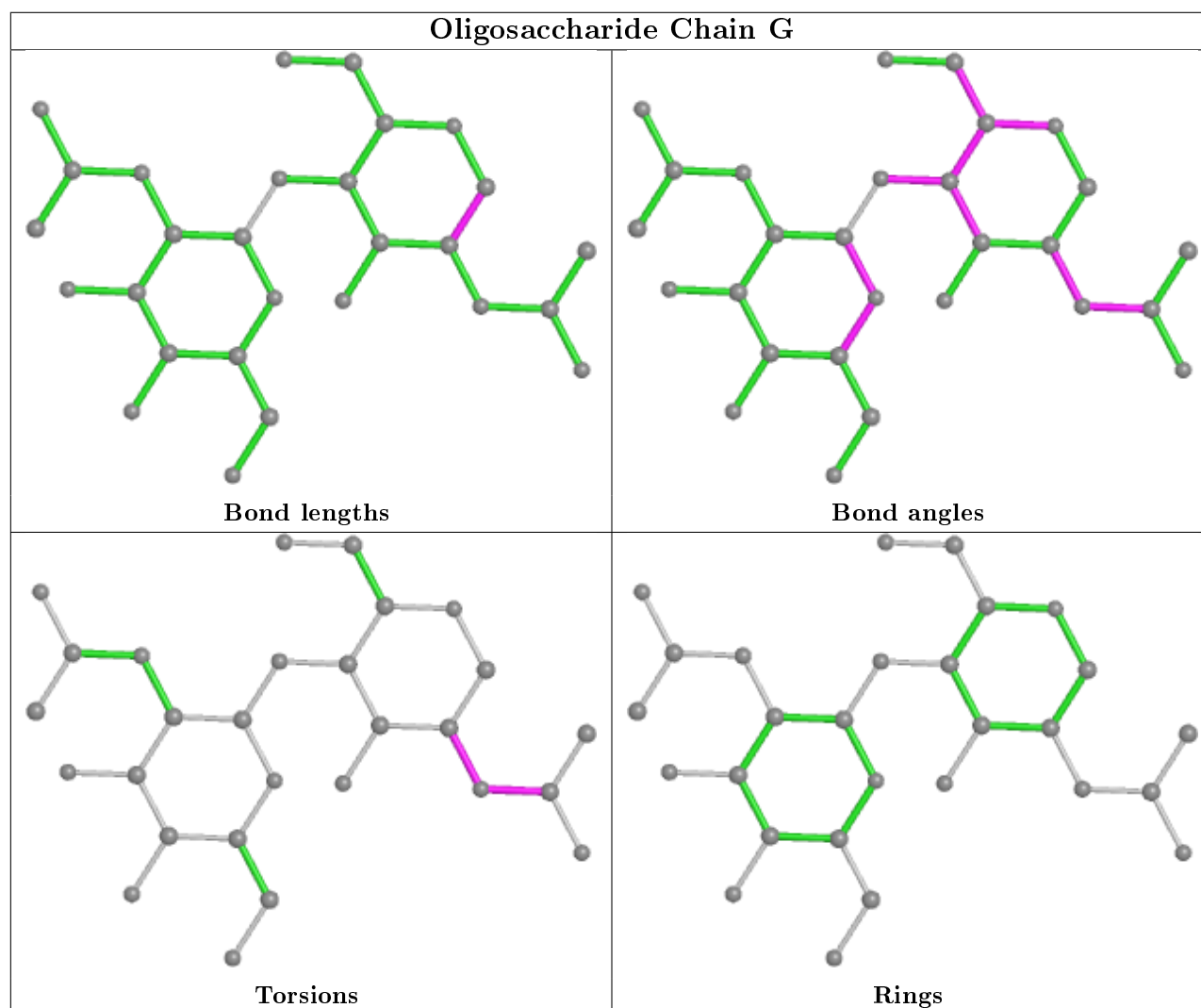
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Mol	Chain	Res	Type	Atoms
4	H	1	NAG	C4-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
5	J	1	NAG	C1-C2-N2-C7
5	J	3	BMA	C4-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
5	J	1	NAG	C8-C7-N2-C2
5	J	1	NAG	O7-C7-N2-C2
4	H	1	NAG	C1-C2-N2-C7
4	H	1	NAG	C3-C2-N2-C7
5	J	1	NAG	C3-C2-N2-C7

There are no ring outliers.

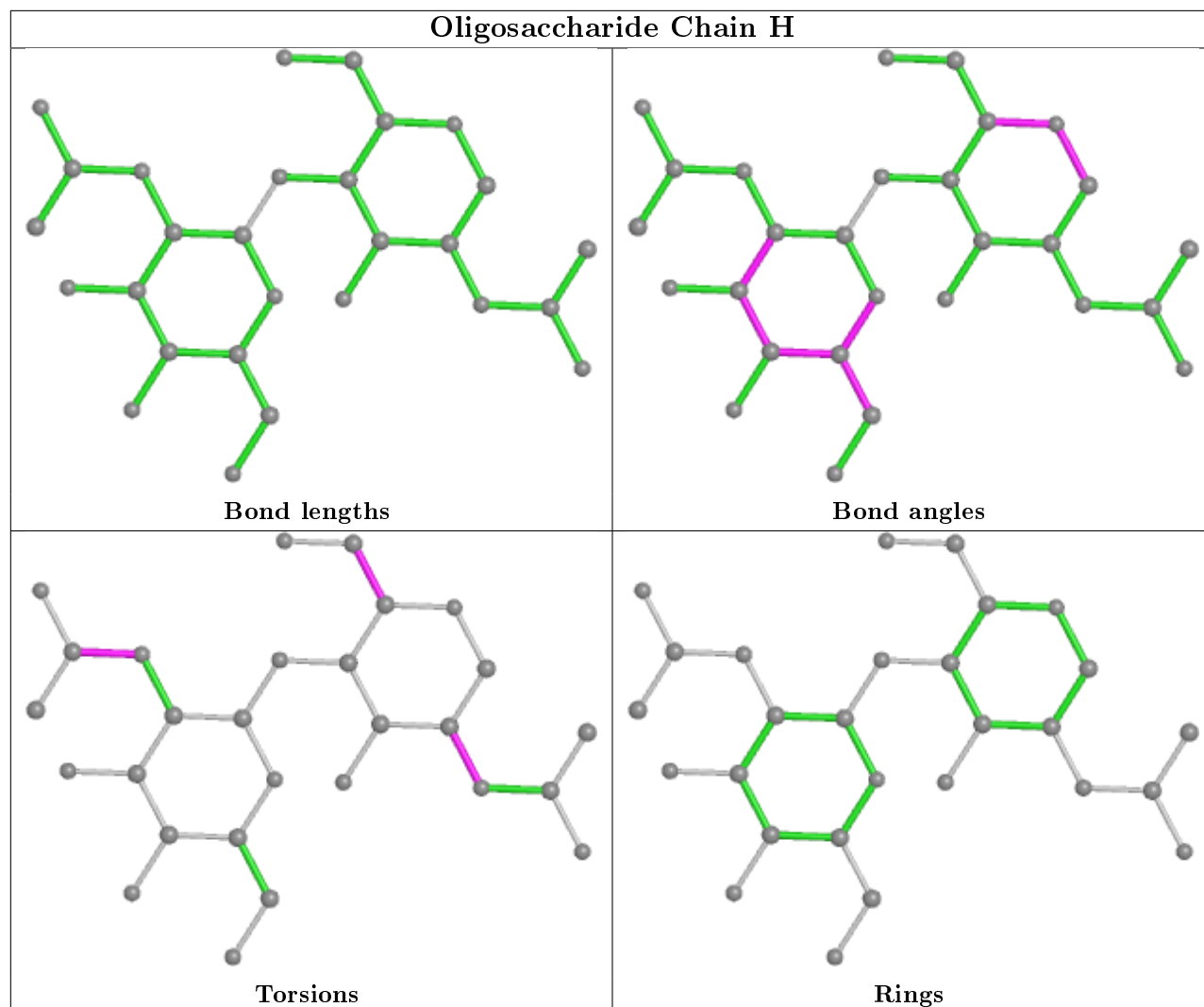
No monomer is involved in short contacts.

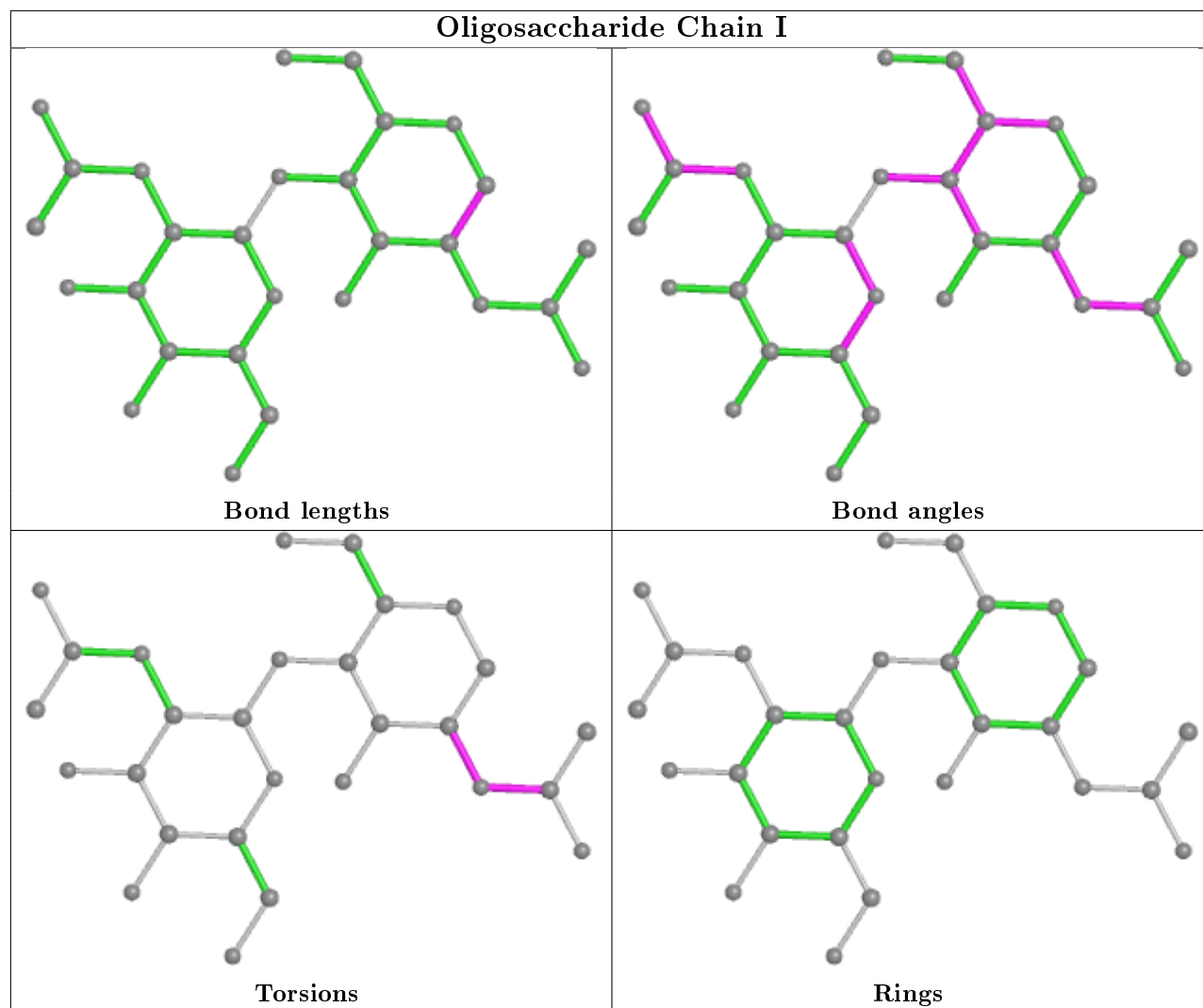
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

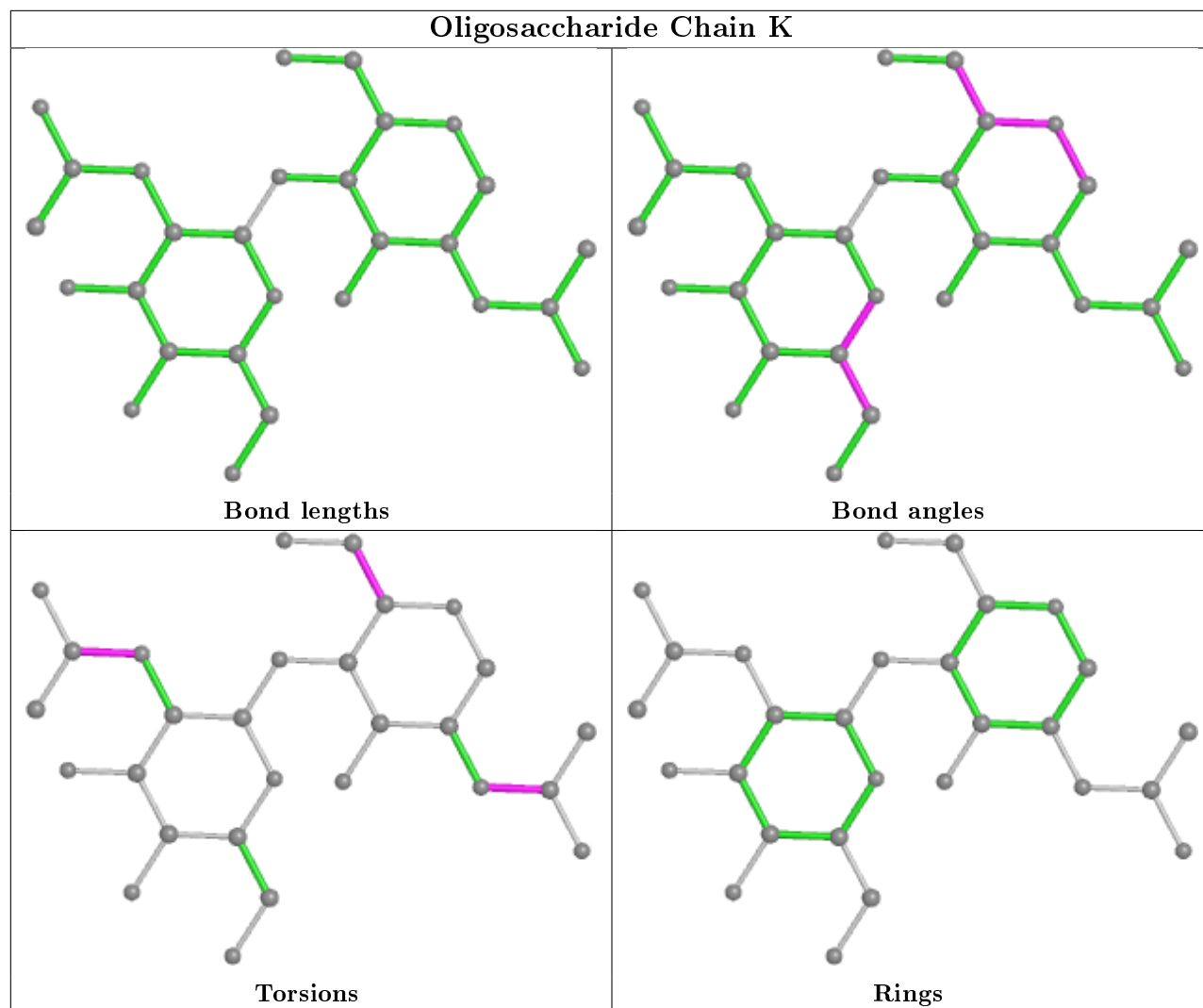


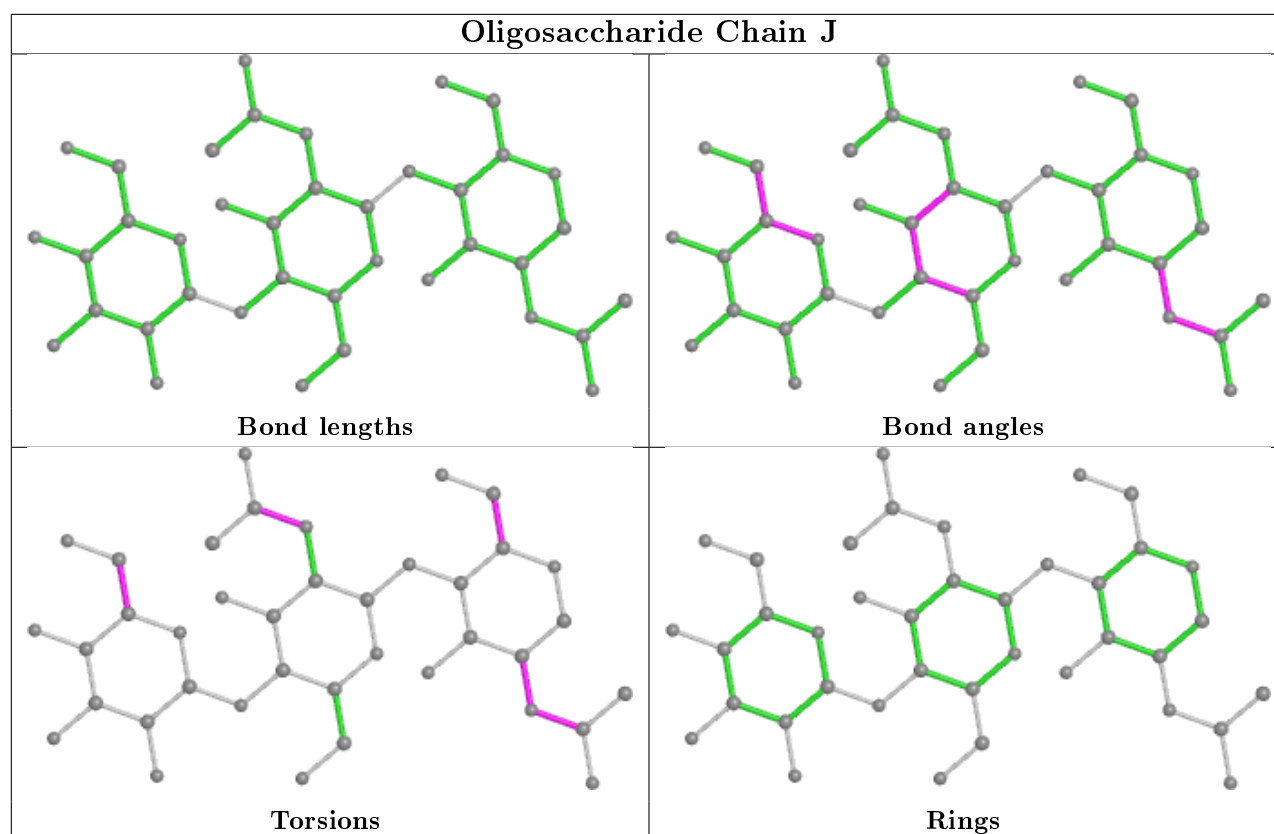


## Oligosaccharide Chain H









## 5.6 Ligand geometry [i](#)

2 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	$\# Z  > 2$
6	NAG	B	1006	1	14,14,15	0.62	0	17,19,21	1.14	2 (11%)
6	NAG	A	1006	1	14,14,15	0.86	0	17,19,21	1.95	6 (35%)

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
6	NAG	B	1006	1	-	3/6/23/26	0/1/1/1
6	NAG	A	1006	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1006	NAG	C1-O5-C5	5.01	118.98	112.19
6	A	1006	NAG	C3-C4-C5	3.46	116.41	110.24
6	B	1006	NAG	C2-N2-C7	2.97	127.13	122.90
6	A	1006	NAG	O5-C1-C2	-2.60	107.18	111.29
6	A	1006	NAG	O5-C5-C4	2.28	116.39	110.83
6	B	1006	NAG	C1-O5-C5	2.25	115.25	112.19
6	A	1006	NAG	C4-C3-C2	2.17	114.20	111.02
6	A	1006	NAG	C6-C5-C4	-2.03	108.24	113.00

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1006	NAG	C8-C7-N2-C2
6	B	1006	NAG	O7-C7-N2-C2
6	A	1006	NAG	C8-C7-N2-C2
6	A	1006	NAG	O7-C7-N2-C2
6	A	1006	NAG	C3-C2-N2-C7
6	B	1006	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	555/624 (88%)	-0.19	20 (3%) 42 39	3, 10, 13, 25	0
1	B	568/624 (91%)	-0.16	12 (2%) 63 61	3, 10, 13, 24	0
2	C	214/214 (100%)	0.51	34 (15%) 1 2	2, 10, 17, 26	0
2	E	214/214 (100%)	-0.31	2 (0%) 84 84	2, 10, 18, 24	0
3	D	222/226 (98%)	0.52	24 (10%) 5 6	2, 10, 17, 32	0
3	F	222/226 (98%)	-0.07	9 (4%) 37 34	2, 11, 19, 29	0
All	All	1995/2128 (93%)	-0.03	101 (5%) 28 26	2, 10, 16, 32	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	128	SER	18.6
3	F	130	SER	10.2
3	D	130	SER	8.1
2	C	193	ALA	7.4
2	C	130	ALA	7.2
2	C	208	SER	6.9
2	C	119	PRO	6.6
2	C	187	GLU	6.2
1	A	544	GLU	6.1
2	C	212	GLY	6.0
3	D	125	ALA	5.7
2	C	196	VAL	5.5
2	C	129	THR	5.3
3	D	216	CYS	5.0
3	D	127	SER	4.9
2	E	214	CYS	4.9
2	C	194	CYS	4.7
2	C	131	SER	4.5
2	C	120	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	545	CYS	4.3
3	D	215	SER	4.2
1	A	546	GLN	4.1
3	D	129	LYS	4.1
2	C	192	TYR	4.0
3	D	214	LYS	3.9
3	D	139	GLY	3.8
3	D	140	CYS	3.8
1	A	547	PRO	3.8
2	C	214	CYS	3.7
3	D	206	LYS	3.7
2	C	181	LEU	3.6
1	B	180	SER	3.6
2	C	186	TYR	3.5
1	A	563	VAL	3.4
2	E	212	GLY	3.4
1	A	543	PRO	3.4
3	D	158	ALA	3.4
2	C	211	ARG	3.3
3	D	199	ASN	3.3
2	C	180	THR	3.3
1	B	576	ALA	3.2
3	D	185	PRO	3.1
3	F	207	VAL	3.1
1	A	562	CYS	3.1
3	F	146	PHE	3.0
3	F	132	SER	2.9
1	B	577	ARG	2.8
3	D	141	LEU	2.8
3	D	179	SER	2.8
1	A	564	ALA	2.8
1	A	557	PRO	2.8
3	D	156	SER	2.8
3	D	204	ASN	2.7
2	C	188	LYS	2.7
2	C	122	ASP	2.7
1	A	197	VAL	2.6
2	C	116	PHE	2.6
3	D	160	THR	2.5
3	D	184	VAL	2.5
2	C	178	THR	2.5
1	A	513	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
3	F	117	LYS	2.5
2	C	148	TRP	2.5
1	B	574	CYS	2.4
1	A	1	THR	2.4
3	D	208	ASP	2.4
2	C	117	ILE	2.4
2	C	158	ASN	2.4
1	B	303	GLU	2.4
1	A	555	PHE	2.3
1	B	318	ARG	2.3
3	F	216	CYS	2.3
1	B	540	PRO	2.3
1	B	572	PRO	2.3
3	F	119	PRO	2.3
3	D	187	SER	2.3
2	C	121	SER	2.3
3	F	118	GLY	2.2
1	A	542	HIS	2.2
2	C	179	LEU	2.2
1	B	568	TYR	2.2
2	C	132	VAL	2.2
1	B	566	ALA	2.2
2	C	118	PHE	2.2
2	C	197	THR	2.2
1	A	536	ARG	2.1
1	A	180	SER	2.1
2	C	205	VAL	2.1
3	F	131	THR	2.1
2	C	124	GLN	2.1
2	C	154	LEU	2.1
3	D	202	PRO	2.1
1	B	570	ASP	2.1
2	C	213	GLU	2.1
1	A	550	GLY	2.1
1	A	512	PHE	2.0
1	A	534	ASN	2.0
3	D	142	VAL	2.0
1	B	573	PHE	2.0
1	A	561	GLN	2.0
2	C	149	LYS	2.0



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

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

## 6.3 Carbohydrates ⓘ

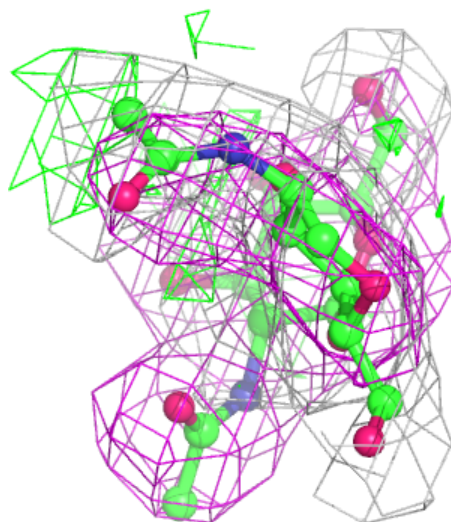
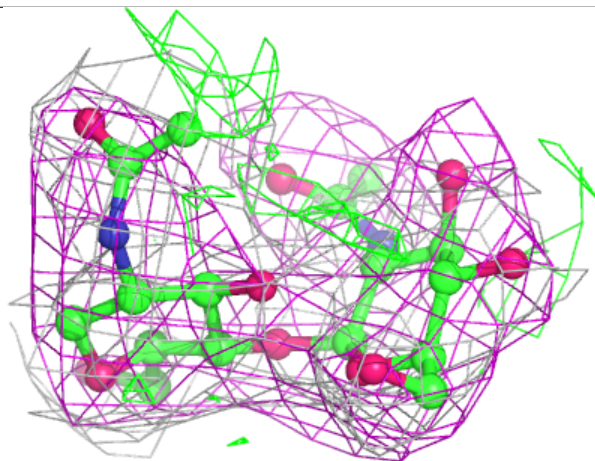
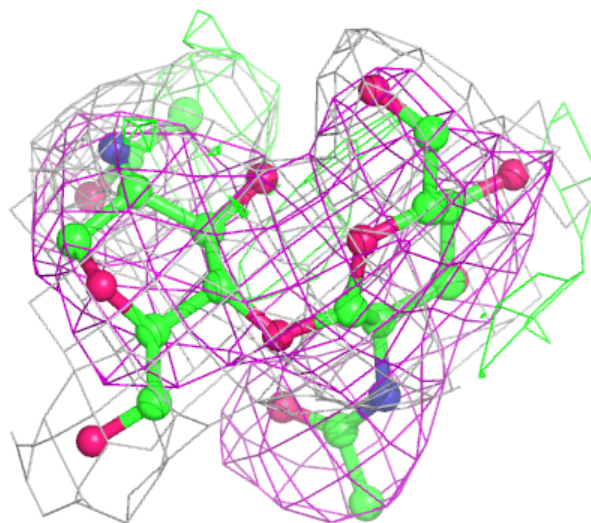
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	J	2	14/15	0.72	0.54	13,15,18,19	0
4	NAG	G	2	14/15	0.74	0.57	11,15,19,20	0
4	NAG	H	2	14/15	0.75	0.53	12,15,18,19	0
5	BMA	J	3	11/12	0.75	0.41	19,23,28,30	0
4	NAG	I	2	14/15	0.79	0.65	11,15,19,20	0
4	NAG	G	1	14/15	0.81	0.39	8,11,13,14	0
4	NAG	K	2	14/15	0.82	0.54	10,11,12,12	0
5	NAG	J	1	14/15	0.86	0.37	8,11,14,14	0
4	NAG	I	1	14/15	0.88	0.29	8,11,13,14	0
4	NAG	K	1	14/15	0.89	0.40	6,9,12,12	0
4	NAG	H	1	14/15	0.91	0.33	8,11,14,15	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.

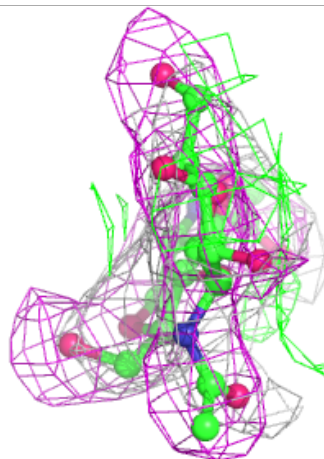
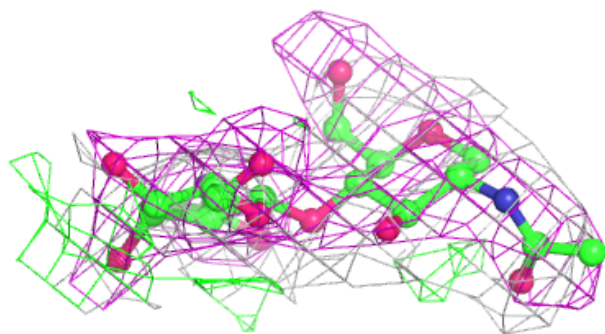
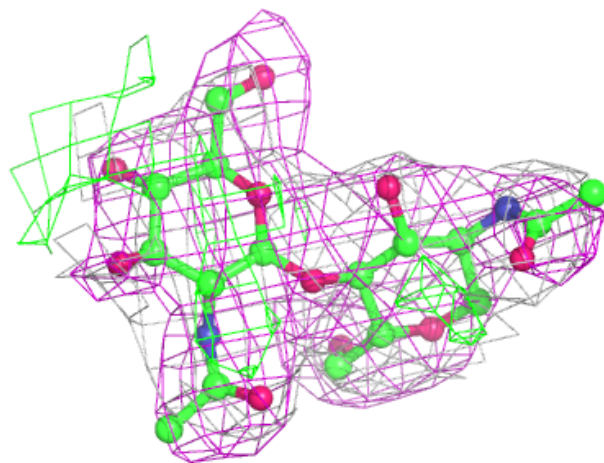
**Electron density around Chain G:**

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



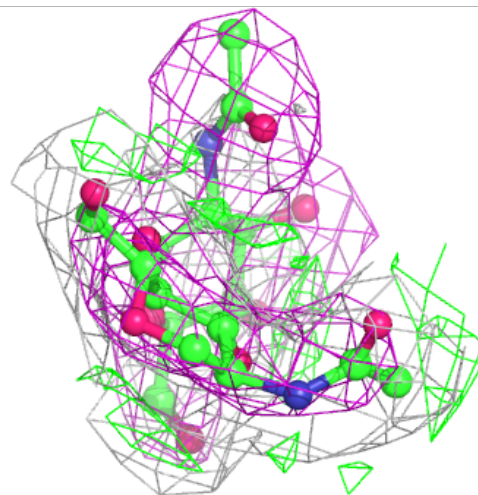
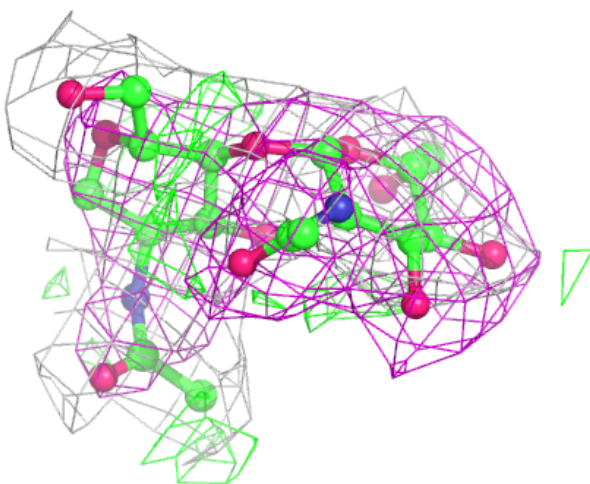
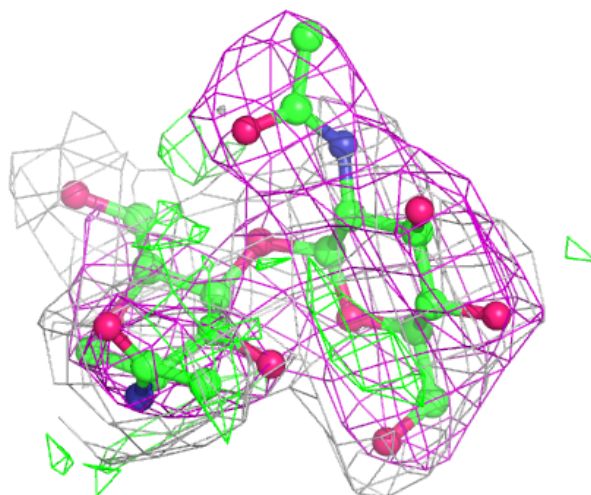
**Electron density around Chain H:**

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



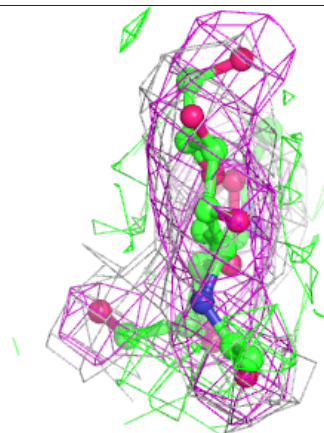
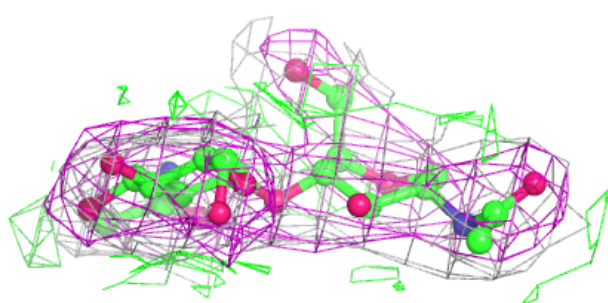
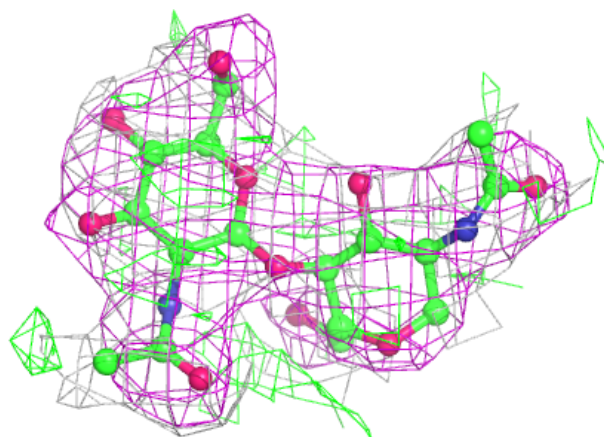
**Electron density around Chain I:**

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

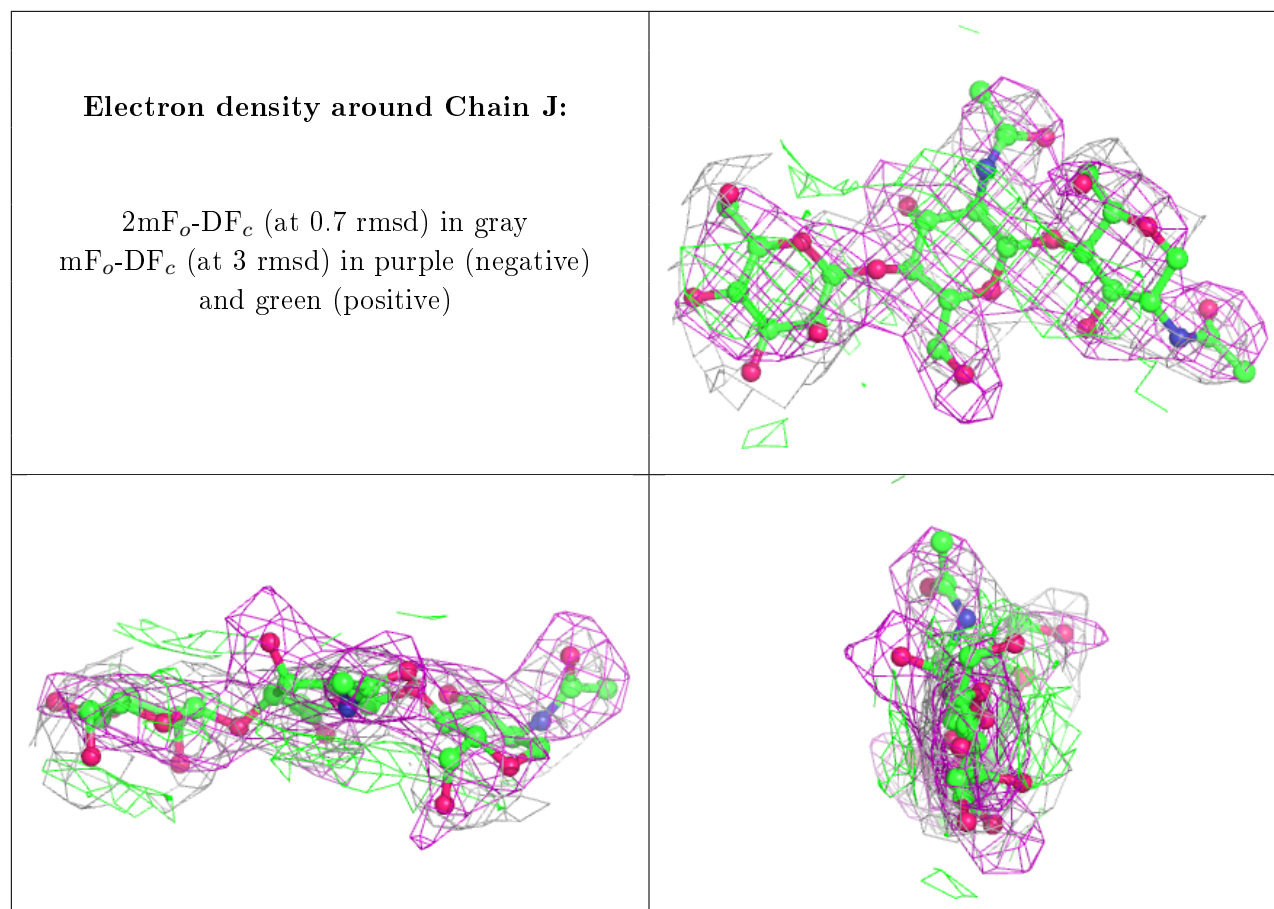


**Electron density around Chain K:**

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







## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	NAG	A	1006	14/15	0.68	0.71	57,68,71,71	0
6	NAG	B	1006	14/15	0.90	0.42	54,64,67,67	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.