



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 02:08 PM UTC

PDB ID : 3E80 / pdb_00003e80
Title : Structure of Heparinase II complexed with heparan sulfate degradation disaccharide product
Authors : Shaya, D.; Cygler, M.
Deposited on : 2008-08-19
Resolution : 2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

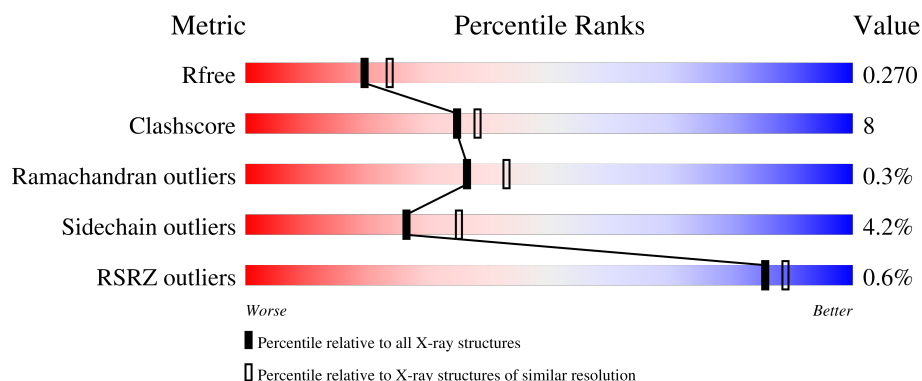
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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.



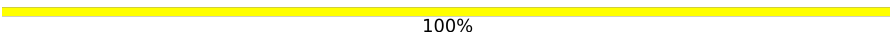
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	749	80% 19% .
1	B	749	% 82% 16% .
1	C	749	% 77% 20% .
2	D	4	100%
2	E	4	100%

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Mol	Chain	Length	Quality of chain
2	F	4	 25% 75%
3	G	2	 100%
3	H	2	 50% 50%
3	I	2	 50% 50%

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
2	XY5	E	3	X	-	-	-
2	GCU	F	2	X	-	-	-
5	PO4	C	6	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 18716 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.

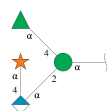
- Molecule 1 is a protein called Heparinase II protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	747	Total	C	N	O	S	0	0	0
			5978	3850	1008	1097	23			
1	B	747	Total	C	N	O	S	0	0	0
			5978	3850	1008	1097	23			
1	C	747	Total	C	N	O	S	0	0	0
			5975	3847	1008	1097	23			

There are 3 discrepancies between the modelled and reference sequences:

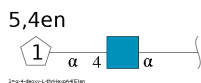
Chain	Residue	Modelled	Actual	Comment	Reference
A	758	ALA	PRO	SEE REMARK 999	UNP Q46080
B	758	ALA	PRO	SEE REMARK 999	UNP Q46080
C	758	ALA	PRO	SEE REMARK 999	UNP Q46080

- Molecule 2 is an oligosaccharide called alpha-D-xylopyranose-(1-4)-alpha-D-glucopyranuronic acid-(1-2)-[alpha-L-rhamnopyranose-(1-4)]alpha-D-mannopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	D	4	Total	C	O	0	0	0
			41	23	18			
2	E	4	Total	C	O	0	0	0
			41	23	18			
2	F	4	Total	C	O	0	0	0
			41	23	18			

- Molecule 3 is an oligosaccharide called 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose.

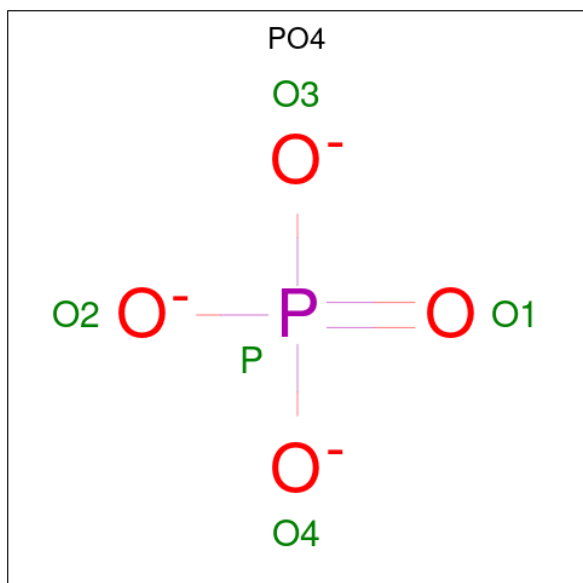


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	2	Total	C	N	O	0	0	0
			26	14	1	11			
3	H	2	Total	C	N	O	0	0	0
			26	14	1	11			
3	I	2	Total	C	N	O	0	0	0
			26	14	1	11			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	A	1	Total	O	P	0	0
			5	4	1		
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		

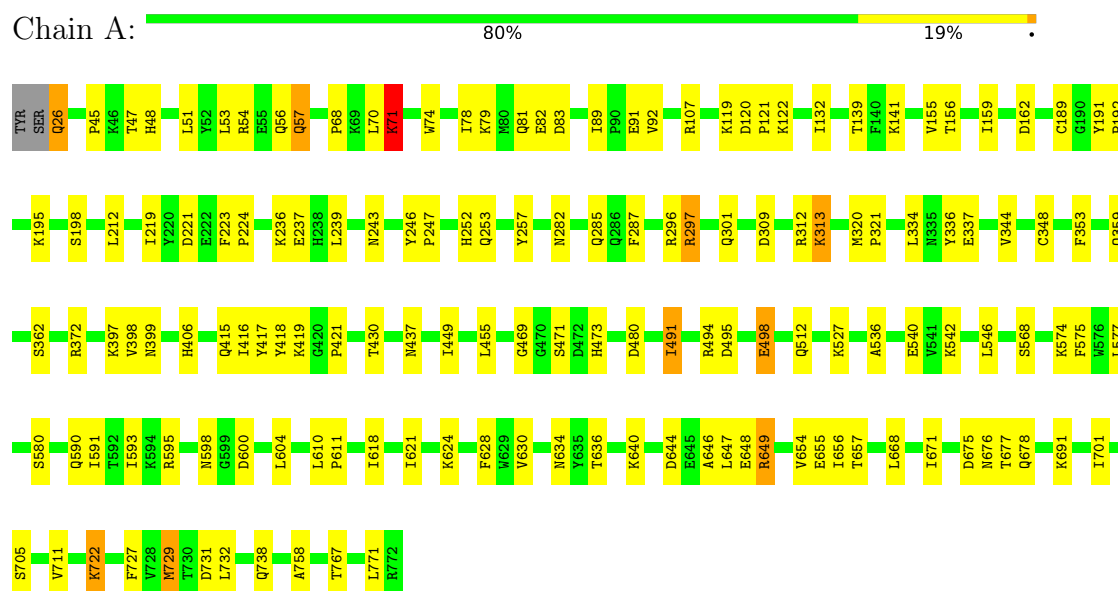
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	208	Total	O	0	0
			208	208		
6	B	151	Total	O	0	0
			151	151		
6	C	177	Total	O	0	0
			177	177		

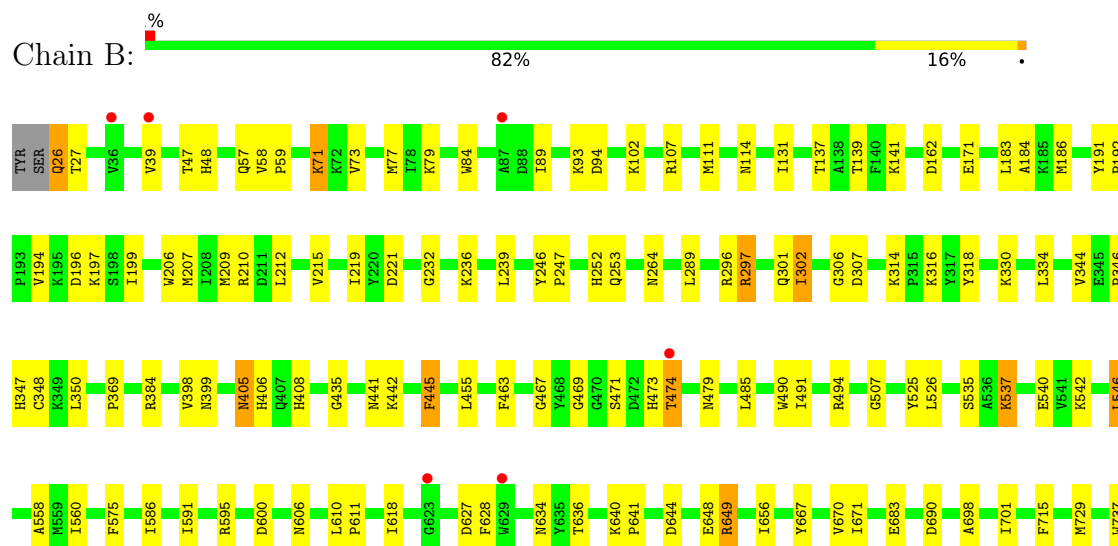
3 Residue-property plots

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: Heparinase II protein



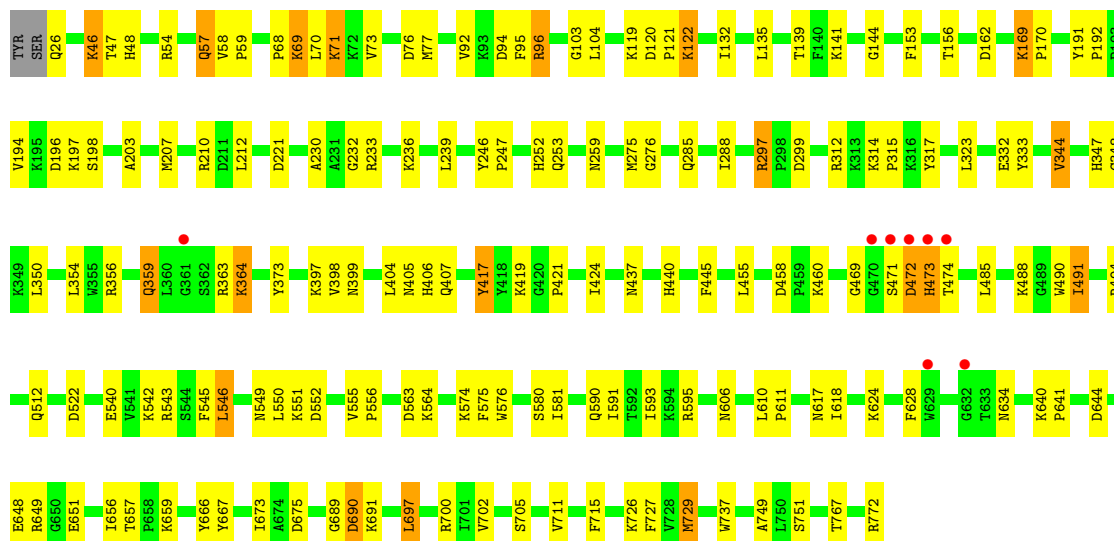
• Molecule 1: Heparinase II protein





- Molecule 1: Heparinase II protein

Chain C: 77% 20%



- Molecule 2: alpha-D-xylopyranose-(1-4)-alpha-D-glucopyranuronic acid-(1-2)-[alpha-L-rhamnopranose-(1-4)]alpha-D-mannopyranose

Chain D: 100%



- Molecule 2: alpha-D-xylopyranose-(1-4)-alpha-D-glucopyranuronic acid-(1-2)-[alpha-L-rhamnopranose-(1-4)]alpha-D-mannopyranose

Chain E: 100%

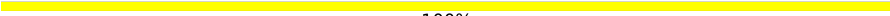


- Molecule 2: alpha-D-xylopyranose-(1-4)-alpha-D-glucopyranuronic acid-(1-2)-[alpha-L-rhamnopranose-(1-4)]alpha-D-mannopyranose

Chain F: 25% 75%



- Molecule 3: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose

Chain G:  100%

HDG1
GCG2

- Molecule 3: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose

Chain H:  50% 50%

HDG1
GCG2

- Molecule 3: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose

Chain I:  50% 50%

HDG1
GCG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	201.28Å 209.36Å 59.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.57 – 2.35 37.57 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.0 (37.57-2.35) 98.0 (37.57-2.35)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.85 (at 2.34Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.229 , 0.267 0.230 , 0.270	Depositor DCC
R_{free} test set	5152 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	18716	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.28 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8089e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PCA, RAM, NDG, XYS, MAN, PO4, GCD, GCU, ZN

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	0.64	0/6133	1.01	11/8303 (0.1%)
1	B	0.58	0/6133	0.99	7/8303 (0.1%)
1	C	0.62	0/6130	1.01	11/8299 (0.1%)
All	All	0.61	0/18396	1.00	29/24905 (0.1%)

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.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	26	PCA	O-C-N	-11.72	104.24	123.00
1	A	26	PCA	O-C-N	-10.30	106.52	123.00
1	B	26	PCA	CA-C-N	-9.63	104.37	121.70
1	B	26	PCA	C-N-CA	-9.63	104.37	121.70
1	C	26	PCA	O-C-N	-8.61	109.23	123.00
1	C	26	PCA	CA-C-N	-6.63	109.77	121.70
1	C	26	PCA	C-N-CA	-6.63	109.77	121.70
1	A	758	ALA	N-CA-C	6.32	119.48	109.50
1	A	79	LYS	N-CA-C	-6.11	104.70	111.36
1	B	507	GLY	N-CA-C	5.83	119.11	110.42
1	C	689	GLY	N-CA-C	5.48	119.20	111.42
1	A	89	ILE	CA-C-N	5.40	125.04	119.05
1	A	89	ILE	C-N-CA	5.40	125.04	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	698	ALA	CB-CA-C	-5.39	110.35	116.54
1	C	491	ILE	CB-CA-C	-5.24	102.43	110.50
1	C	169	LYS	CB-CA-C	5.22	116.98	109.09
1	C	397	LYS	N-CA-C	5.22	117.94	109.06
1	C	207	MET	N-CA-C	5.21	117.64	111.33
1	C	690	ASP	N-CA-C	-5.20	100.30	108.63
1	B	131	ILE	N-CA-C	5.19	116.10	111.90
1	A	649	ARG	N-CA-C	-5.19	106.90	113.18
1	C	132	ILE	N-CA-C	5.18	116.64	111.00
1	A	132	ILE	N-CA-C	5.15	115.92	110.72
1	B	445	PHE	N-CA-C	5.13	117.28	111.02
1	C	424	ILE	N-CA-C	5.12	117.06	109.17
1	A	71	LYS	N-CA-C	-5.07	105.40	111.03
1	A	397	LYS	N-CA-C	5.07	116.65	108.34
1	A	491	ILE	CB-CA-C	-5.03	102.86	110.95
1	A	495	ASP	N-CA-C	5.01	114.76	108.45

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	26	PCA	Mainchain

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	5978	0	5889	91	0
1	B	5978	0	5889	75	0
1	C	5975	0	5880	104	0
2	D	41	0	29	0	0
2	E	41	0	30	1	0
2	F	41	0	29	0	0
3	G	26	0	16	0	0
3	H	26	0	16	1	0
3	I	26	0	16	2	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	20	0	0	0	0
5	B	15	0	0	0	0
5	C	10	0	0	3	0
6	A	208	0	0	9	0
6	B	151	0	0	4	0
6	C	177	0	0	7	0
All	All	18716	0	17794	271	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 (271) 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:B:253:GLN:HE22	1:B:405:ASN:HB3	1.26	0.98
1:C:574:LYS:O	1:C:657:THR:HG22	1.74	0.87
1:C:253:GLN:HE22	1:C:405:ASN:HB3	1.46	0.79
1:A:54:ARG:H	1:A:57:GLN:HE21	1.26	0.79
1:B:628:PHE:H	1:B:634:ASN:HD21	1.33	0.74
1:A:253:GLN:HE22	1:A:406:HIS:H	1.36	0.73
1:C:419:LYS:HE2	1:C:675:ASP:OD1	1.88	0.73
1:A:83:ASP:OD1	1:A:107:ARG:NH2	2.21	0.73
1:B:209:MET:HE3	1:B:264:ASN:HB3	1.70	0.72
1:A:81:GLN:HE21	1:A:107:ARG:HA	1.52	0.72
1:A:628:PHE:H	1:A:634:ASN:HD21	1.36	0.72
1:A:727:PHE:HB3	1:A:729:MET:HE3	1.71	0.71
1:C:628:PHE:H	1:C:634:ASN:HD21	1.37	0.71
1:C:344:VAL:HG13	1:C:348:CYS:HB2	1.71	0.71
1:C:48:HIS:HD2	1:C:162:ASP:OD1	1.72	0.71
1:C:455:LEU:HB2	1:C:575:PHE:HB2	1.73	0.70
1:B:26:PCA:OE	1:B:330:LYS:NZ	2.21	0.70
1:B:535:SER:OG	1:B:537:LYS:HD3	1.92	0.69
1:B:369:PRO:HG2	1:C:749:ALA:HB3	1.75	0.69
1:B:253:GLN:HE22	1:B:406:HIS:H	1.41	0.68
1:C:474:THR:HG23	1:C:474:THR:O	1.92	0.68
1:A:74:TRP:CZ2	1:A:78:ILE:HD11	2.28	0.68
1:C:610:LEU:HA	1:C:611:PRO:C	2.19	0.68
1:B:442:LYS:NZ	1:B:474:THR:HB	2.09	0.66
1:B:79:LYS:HE3	6:B:817:HOH:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:MET:HB2	1:A:732:LEU:HD11	1.78	0.65
1:B:48:HIS:HD2	1:B:162:ASP:OD1	1.78	0.65
1:B:210:ARG:HH12	1:B:347:HIS:HD2	1.44	0.65
1:C:690:ASP:HA	6:C:848:HOH:O	1.96	0.65
1:B:455:LEU:HB2	1:B:575:PHE:HB2	1.78	0.64
1:C:540:GLU:OE2	1:C:542:LYS:HE2	1.98	0.64
1:C:70:LEU:O	1:C:73:VAL:HG12	1.97	0.63
1:B:210:ARG:HH12	1:B:347:HIS:CD2	2.16	0.63
1:B:253:GLN:NE2	1:B:405:ASN:HB3	2.06	0.63
1:C:437:ASN:ND2	1:C:471:SER:HB3	2.14	0.62
1:A:540:GLU:OE2	1:A:542:LYS:HE2	2.00	0.62
1:B:77:MET:HE1	1:B:350:LEU:HB2	1.82	0.61
1:B:297:ARG:NH2	1:B:648:GLU:OE1	2.32	0.61
1:B:610:LEU:HA	1:B:611:PRO:C	2.25	0.61
1:B:302:ILE:HG13	1:B:316:LYS:HE3	1.82	0.61
1:A:282:ASN:HB2	6:A:906:HOH:O	1.99	0.61
1:B:469:GLY:O	1:B:473:HIS:HE1	1.84	0.61
1:C:727:PHE:HB3	1:C:729:MET:HE3	1.84	0.60
1:A:313:LYS:HG3	6:A:802:HOH:O	2.00	0.60
1:C:54:ARG:HH12	1:C:276:GLY:HA3	1.67	0.60
1:A:644:ASP:OD2	1:A:649:ARG:HD2	2.03	0.59
5:C:6:PO4:O4	3:I:2:GCD:H4	2.02	0.59
1:A:455:LEU:HB2	1:A:575:PHE:HB2	1.84	0.59
1:B:442:LYS:HZ1	1:B:474:THR:HB	1.65	0.59
1:C:197:LYS:O	1:C:203:ALA:HB3	2.03	0.58
1:C:119:LYS:HE2	6:C:811:HOH:O	2.03	0.58
1:C:95:PHE:CZ	5:C:6:PO4:O1	2.56	0.58
1:A:54:ARG:N	1:A:57:GLN:HE21	2.00	0.57
1:C:697:LEU:O	1:C:697:LEU:HD23	2.03	0.57
1:A:74:TRP:CH2	1:A:78:ILE:HD11	2.39	0.57
1:A:219:ILE:HD12	1:A:223:PHE:HB3	1.87	0.57
1:B:535:SER:HG	1:B:537:LYS:HD3	1.68	0.57
1:A:580:SER:HB3	1:A:593:ILE:HD13	1.87	0.56
1:B:525:TYR:HB2	1:B:546:LEU:HD12	1.88	0.56
1:A:57:GLN:NE2	6:A:905:HOH:O	2.36	0.56
1:B:194:VAL:O	1:B:494:ARG:NH1	2.36	0.56
1:B:595:ARG:NH1	1:B:600:ASP:OD2	2.39	0.56
1:C:315:PRO:HB2	1:C:317:TYR:CZ	2.42	0.55
1:A:621:ILE:HD12	1:A:655:GLU:OE2	2.07	0.55
1:B:58:VAL:HB	1:B:59:PRO:HD3	1.87	0.55
1:C:364:LYS:H	1:C:364:LYS:CD	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:TYR:CE2	1:A:285:GLN:HG3	2.41	0.55
1:C:737:TRP:CE2	1:C:772:ARG:HD3	2.41	0.55
1:B:207:MET:O	1:B:212:LEU:HB2	2.07	0.55
1:A:398:VAL:O	1:A:399:ASN:HB2	2.06	0.55
1:C:691:LYS:HE3	6:C:911:HOH:O	2.05	0.55
1:A:344:VAL:CG1	1:A:348:CYS:HB2	2.37	0.55
1:A:722:LYS:HA	1:A:722:LYS:HE3	1.87	0.55
1:A:68:PRO:HA	1:A:71:LYS:HB2	1.88	0.54
1:C:54:ARG:H	1:C:57:GLN:HE21	1.54	0.54
1:C:522:ASP:HB3	1:C:700:ARG:NH1	2.22	0.54
1:C:210:ARG:HH12	1:C:347:HIS:HD2	1.53	0.54
1:B:79:LYS:HE2	6:B:900:HOH:O	2.06	0.54
1:C:564:LYS:HG3	1:C:666:TYR:CE2	2.43	0.54
1:B:485:LEU:HD22	1:B:490:TRP:CE2	2.42	0.54
1:C:580:SER:HB3	1:C:593:ILE:HD13	1.90	0.54
1:B:206:TRP:HA	1:B:264:ASN:OD1	2.08	0.54
1:C:253:GLN:HE22	1:C:406:HIS:H	1.56	0.54
1:B:540:GLU:OE2	1:B:542:LYS:HE2	2.08	0.54
1:C:576:TRP:CE3	1:C:656:ILE:HD12	2.42	0.54
1:A:455:LEU:HD11	1:A:577:LEU:HD11	1.91	0.53
1:C:196:ASP:HB3	1:C:203:ALA:HB2	1.91	0.53
1:B:253:GLN:NE2	1:B:406:HIS:H	2.06	0.53
1:A:421:PRO:HD2	1:A:595:ARG:HD2	1.92	0.52
1:B:191:TYR:HA	1:B:192:PRO:C	2.34	0.52
1:C:485:LEU:HD22	1:C:490:TRP:CE2	2.44	0.52
1:C:210:ARG:HH12	1:C:347:HIS:CD2	2.28	0.52
1:A:120:ASP:OD1	1:A:120:ASP:C	2.53	0.52
1:A:344:VAL:HG12	1:A:348:CYS:HB2	1.90	0.52
1:A:312:ARG:HH22	1:A:600:ASP:CG	2.17	0.51
1:C:549:ASN:O	1:C:551:LYS:HG2	2.10	0.51
1:C:546:LEU:HD22	1:C:702:VAL:HG21	1.91	0.51
1:C:618:ILE:HG12	1:C:656:ILE:HG12	1.93	0.51
1:B:467:GLY:O	1:B:491:ILE:HD12	2.11	0.51
1:A:48:HIS:HD2	1:A:162:ASP:OD1	1.94	0.50
1:B:737:TRP:CE2	1:B:772:ARG:HD3	2.46	0.50
1:C:69:LYS:HD3	1:C:69:LYS:H	1.76	0.50
1:C:246:TYR:N	1:C:247:PRO:CD	2.74	0.50
1:A:191:TYR:HA	1:A:192:PRO:C	2.37	0.50
1:A:312:ARG:NH1	1:A:648:GLU:OE2	2.43	0.50
1:B:297:ARG:HH22	1:B:648:GLU:CD	2.18	0.50
1:C:169:LYS:HB2	1:C:170:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ASN:O	1:A:247:PRO:HD3	2.11	0.50
1:A:675:ASP:C	1:A:677:THR:H	2.19	0.50
1:C:246:TYR:CE2	1:C:285:GLN:HB2	2.46	0.50
1:A:336:TYR:HB2	1:A:362:SER:HB2	1.94	0.50
1:C:398:VAL:O	1:C:399:ASN:HB2	2.10	0.50
1:C:469:GLY:O	1:C:473:HIS:CE1	2.65	0.50
1:A:48:HIS:HE1	1:A:221:ASP:OD1	1.95	0.50
1:C:119:LYS:O	1:C:121:PRO:HD3	2.12	0.50
1:C:591:ILE:HD12	1:C:606:ASN:HD22	1.76	0.49
1:A:296:ARG:HH12	1:A:337:GLU:CD	2.20	0.49
1:B:302:ILE:HD12	1:B:318:TYR:HE1	1.78	0.49
1:C:232:GLY:O	1:C:236:LYS:HB2	2.12	0.49
1:C:543:ARG:HD3	1:C:545:PHE:CE2	2.48	0.49
1:B:183:LEU:O	1:B:186:MET:HB2	2.12	0.49
1:C:417:TYR:C	1:C:417:TYR:CD2	2.91	0.49
1:B:628:PHE:HZ	1:B:649:ARG:HG3	1.77	0.49
1:A:297:ARG:NH1	1:A:301:GLN:HB2	2.28	0.49
1:B:618:ILE:HG12	1:B:656:ILE:HG12	1.95	0.48
1:C:54:ARG:NH1	1:C:275:MET:O	2.45	0.48
1:A:189:CYS:O	1:A:195:LYS:HB2	2.13	0.48
1:C:253:GLN:HE22	1:C:405:ASN:CB	2.23	0.48
1:C:58:VAL:N	1:C:59:PRO:CD	2.76	0.48
1:C:54:ARG:NH1	1:C:276:GLY:HA3	2.28	0.48
1:A:512:GLN:NE2	6:A:923:HOH:O	2.43	0.48
1:A:738:GLN:HE21	1:A:771:LEU:HD12	1.77	0.48
1:B:84:TRP:HB3	1:B:89:ILE:HG12	1.96	0.48
1:C:246:TYR:CD2	1:C:285:GLN:HB2	2.49	0.48
1:A:604:LEU:HG	1:A:671:ILE:HG23	1.96	0.48
1:C:705:SER:HB2	1:C:711:VAL:HG23	1.96	0.48
1:B:296:ARG:O	1:B:384:ARG:NH2	2.47	0.47
1:A:527:LYS:NZ	1:A:731:ASP:OD1	2.42	0.47
1:C:121:PRO:HB3	6:C:939:HOH:O	2.13	0.47
5:C:6:PO4:O4	3:I:2:GCD:C4	2.62	0.47
1:B:102:LYS:O	2:E:4:RAM:O3	2.31	0.47
1:B:246:TYR:N	1:B:247:PRO:CD	2.77	0.47
1:B:347:HIS:HE1	6:B:912:HOH:O	1.96	0.47
1:C:48:HIS:HE1	1:C:221:ASP:OD1	1.97	0.47
1:C:73:VAL:O	1:C:76:ASP:HB2	2.15	0.47
1:C:252:HIS:O	1:C:407:GLN:HB2	2.15	0.47
1:C:350:LEU:O	1:C:354:LEU:HG	2.15	0.47
1:A:591:ILE:HD13	1:A:654:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:GLY:O	1:B:236:LYS:HB2	2.14	0.47
1:C:690:ASP:O	1:C:715:PHE:HB2	2.15	0.46
1:A:45:PRO:HB2	1:A:47:THR:HG22	1.96	0.46
1:B:306:GLY:HA2	1:B:408:HIS:CD2	2.50	0.46
1:C:644:ASP:OD2	1:C:649:ARG:HD2	2.15	0.46
1:A:437:ASN:ND2	1:A:471:SER:HB2	2.30	0.46
1:A:610:LEU:HA	1:A:611:PRO:C	2.40	0.46
1:A:618:ILE:HG12	1:A:656:ILE:HG12	1.96	0.46
1:B:690:ASP:O	1:B:715:PHE:HB2	2.16	0.46
1:C:297:ARG:NH1	1:C:299:ASP:OD2	2.48	0.46
1:C:458:ASP:OD1	1:C:458:ASP:C	2.59	0.46
1:A:155:VAL:HG12	1:A:159:ILE:HD11	1.97	0.46
1:A:418:TYR:O	1:A:419:LYS:C	2.56	0.46
1:A:449:ILE:HB	1:A:480:ASP:HB2	1.96	0.46
1:B:627:ASP:OD1	1:B:627:ASP:N	2.48	0.46
1:A:287:PHE:HB3	1:A:372:ARG:NH2	2.31	0.46
1:B:48:HIS:HE1	1:B:221:ASP:OD1	1.98	0.46
1:A:320:MET:N	1:A:321:PRO:CD	2.79	0.45
1:C:297:ARG:NH2	1:C:421:PRO:HG3	2.31	0.45
1:A:595:ARG:HH12	1:A:598:ASN:HD22	1.63	0.45
1:B:644:ASP:OD2	1:B:649:ARG:HD2	2.16	0.45
1:A:54:ARG:HB2	1:A:57:GLN:NE2	2.31	0.45
1:A:494:ARG:HB3	1:A:498:GLU:OE1	2.16	0.45
1:A:574:LYS:O	1:A:657:THR:HG22	2.16	0.45
1:A:640:LYS:H	1:A:640:LYS:HG2	1.59	0.45
1:B:196:ASP:CG	1:B:197:LYS:H	2.24	0.45
1:C:194:VAL:O	1:C:494:ARG:NH1	2.50	0.45
1:C:610:LEU:CA	1:C:611:PRO:C	2.89	0.45
1:A:359:GLN:HB2	6:A:930:HOH:O	2.16	0.45
1:C:94:ASP:OD2	1:C:96:ARG:HG3	2.16	0.45
1:C:198:SER:HG	1:C:233:ARG:HE	1.65	0.45
1:A:252:HIS:CD2	1:A:253:GLN:HG2	2.51	0.45
1:C:191:TYR:HA	1:C:192:PRO:C	2.42	0.45
1:A:705:SER:HB2	1:A:711:VAL:HG23	1.99	0.44
1:A:257:TYR:CE1	1:A:406:HIS:CE1	3.05	0.44
1:A:415:GLN:C	1:A:416:ILE:HG13	2.43	0.44
1:B:640:LYS:O	1:B:641:PRO:C	2.59	0.44
1:C:700:ARG:NE	1:C:726:LYS:HD2	2.33	0.44
1:B:296:ARG:NH2	1:B:316:LYS:O	2.50	0.44
1:B:463:PHE:CE1	1:B:479:ASN:HA	2.53	0.44
1:C:77:MET:HE1	1:C:350:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ASP:OD1	1:C:122:LYS:HD3	2.18	0.44
1:C:323:LEU:HD11	1:C:356:ARG:HB2	2.00	0.44
1:A:449:ILE:HD13	1:A:630:VAL:HG22	1.99	0.44
1:B:560:ILE:HG12	1:B:670:VAL:HG22	2.00	0.44
1:C:404:LEU:HB3	1:C:405:ASN:H	1.71	0.44
1:A:119:LYS:O	1:A:121:PRO:HD3	2.18	0.44
1:B:344:VAL:HG12	1:B:348:CYS:HB2	2.00	0.44
1:C:312:ARG:NH1	1:C:648:GLU:OE2	2.50	0.44
1:B:71:LYS:HA	1:B:71:LYS:HD2	1.57	0.44
1:B:307:ASP:HA	1:B:445:PHE:HE2	1.83	0.44
1:A:236:LYS:HG2	1:A:237:GLU:HG3	2.00	0.43
1:B:591:ILE:HD12	1:B:606:ASN:HD22	1.83	0.43
1:C:617:ASN:HB2	1:C:657:THR:O	2.18	0.43
1:A:70:LEU:HD22	1:A:353:PHE:HA	1.98	0.43
1:C:563:ASP:HB2	1:C:667:TYR:HB2	2.00	0.43
1:A:691:LYS:HD2	6:A:954:HOH:O	2.18	0.43
1:C:246:TYR:CD1	1:C:288:ILE:HD11	2.53	0.43
1:C:47:THR:HB	6:C:941:HOH:O	2.17	0.43
1:C:297:ARG:HH21	1:C:421:PRO:HG3	1.83	0.43
1:C:640:LYS:O	1:C:641:PRO:C	2.61	0.43
1:A:610:LEU:HB2	1:A:668:LEU:HB3	1.99	0.43
1:B:289:LEU:HB3	1:B:334:LEU:HD22	2.01	0.43
1:A:536:ALA:O	1:A:568:SER:OG	2.32	0.43
1:A:628:PHE:H	1:A:634:ASN:ND2	2.11	0.43
1:A:198:SER:OG	1:A:237:GLU:OE1	2.25	0.43
1:A:224:PRO:HD2	6:A:821:HOH:O	2.18	0.43
1:C:196:ASP:CG	1:C:197:LYS:H	2.27	0.43
1:A:598:ASN:ND2	1:A:646:ALA:HA	2.34	0.43
1:C:333:TYR:CZ	1:C:363:ARG:HD2	2.54	0.43
1:C:617:ASN:HD21	1:C:659:LYS:HD3	1.84	0.43
1:A:120:ASP:O	1:A:121:PRO:C	2.61	0.43
1:A:678:GLN:HA	1:A:678:GLN:NE2	2.34	0.43
1:A:598:ASN:HD21	1:A:646:ALA:HA	1.83	0.42
1:B:184:ALA:C	1:B:186:MET:H	2.25	0.42
1:A:334:LEU:O	1:A:337:GLU:HB3	2.20	0.42
1:C:212:LEU:HG	1:C:230:ALA:HB2	2.00	0.42
1:A:469:GLY:O	1:A:473:HIS:HE1	2.02	0.42
1:B:93:LYS:HB2	6:B:816:HOH:O	2.20	0.42
1:C:46:LYS:NZ	1:C:46:LYS:HB2	2.34	0.42
1:A:51:LEU:C	1:A:53:LEU:H	2.27	0.42
1:B:586:ILE:HD13	1:B:618:ILE:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:558:ALA:HA	1:B:671:ILE:O	2.20	0.42
1:B:435:GLY:O	1:B:441:ASN:ND2	2.50	0.42
1:B:215:VAL:O	1:B:219:ILE:HG12	2.19	0.42
1:B:252:HIS:CD2	1:B:253:GLN:HG2	2.55	0.42
1:B:297:ARG:HD2	1:B:301:GLN:HB2	2.01	0.42
1:B:405:ASN:ND2	3:H:1:NDG:C7	2.82	0.42
1:C:103:GLY:O	1:C:104:LEU:C	2.62	0.42
1:C:153:PHE:O	1:C:156:THR:HB	2.20	0.41
1:C:373:TYR:CZ	1:C:512:GLN:HG2	2.55	0.41
1:A:155:VAL:O	1:A:156:THR:C	2.63	0.41
1:B:306:GLY:HA2	1:B:408:HIS:CE1	2.55	0.41
1:A:212:LEU:HD12	1:A:212:LEU:HA	1.79	0.41
1:A:542:LYS:NZ	6:A:795:HOH:O	2.49	0.41
1:B:610:LEU:O	1:B:667:TYR:HA	2.21	0.41
1:C:440:HIS:CD2	1:C:445:PHE:HB2	2.56	0.41
1:A:297:ARG:HG2	1:A:417:TYR:CE1	2.56	0.41
1:A:309:ASP:OD2	1:A:430:THR:OG1	2.32	0.41
1:A:675:ASP:C	1:A:677:THR:N	2.79	0.41
1:B:307:ASP:HA	1:B:445:PHE:CE2	2.56	0.41
1:C:47:THR:HG22	1:C:48:HIS:N	2.36	0.41
1:C:252:HIS:CE1	6:C:784:HOH:O	2.74	0.41
1:C:314:LYS:O	1:C:315:PRO:C	2.64	0.41
1:C:332:GLU:HG3	6:C:907:HOH:O	2.21	0.41
1:C:581:ILE:O	1:C:651:GLU:HB2	2.21	0.41
1:A:647:LEU:HD12	1:A:649:ARG:HD3	2.02	0.41
1:B:772:ARG:O	1:B:772:ARG:HG3	2.22	0.41
1:C:474:THR:O	1:C:474:THR:CG2	2.64	0.41
1:C:550:LEU:HD12	1:C:555:VAL:O	2.21	0.40
1:A:74:TRP:CE2	1:A:78:ILE:HD11	2.57	0.40
1:A:595:ARG:NH2	6:A:931:HOH:O	2.54	0.40
1:C:135:LEU:HA	1:C:153:PHE:CE2	2.56	0.40
1:C:419:LYS:CE	1:C:675:ASP:OD1	2.63	0.40
1:A:246:TYR:CZ	1:A:285:GLN:HG3	2.56	0.40
1:B:398:VAL:HG23	1:B:526:LEU:HD21	2.03	0.40
1:C:556:PRO:HD2	1:C:673:ILE:O	2.21	0.40
1:A:678:GLN:HA	1:A:678:GLN:HE21	1.86	0.40
1:B:107:ARG:O	1:B:111:MET:HG3	2.21	0.40
1:C:48:HIS:CD2	1:C:162:ASP:OD1	2.62	0.40
1:C:54:ARG:H	1:C:57:GLN:NE2	2.20	0.40
1:C:68:PRO:O	1:C:71:LYS:HB2	2.21	0.40
1:C:359:GLN:HA	1:C:359:GLN:NE2	2.37	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	745/749 (100%)	696 (93%)	47 (6%)	2 (0%)	36	43
1	B	745/749 (100%)	695 (93%)	49 (7%)	1 (0%)	48	59
1	C	745/749 (100%)	694 (93%)	48 (6%)	3 (0%)	30	34
All	All	2235/2247 (100%)	2085 (93%)	144 (6%)	6 (0%)	36	43

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	472	ASP
1	A	91	GLU
1	B	399	ASN
1	C	473	HIS
1	A	676	ASN
1	C	144	GLY

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	632/634 (100%)	611 (97%)	21 (3%)	33	44
1	B	632/634 (100%)	603 (95%)	29 (5%)	24	31
1	C	631/634 (100%)	602 (95%)	29 (5%)	24	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1895/1902 (100%)	1816 (96%)	79 (4%)	26	35

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	57	GLN
1	A	71	LYS
1	A	82	GLU
1	A	92	VAL
1	A	122	LYS
1	A	139	THR
1	A	141	LYS
1	A	239	LEU
1	A	297	ARG
1	A	313	LYS
1	A	491	ILE
1	A	498	GLU
1	A	546	LEU
1	A	590	GLN
1	A	624	LYS
1	A	636	THR
1	A	701	ILE
1	A	722	LYS
1	A	729	MET
1	A	767	THR
1	B	27	THR
1	B	39	VAL
1	B	47	THR
1	B	57	GLN
1	B	71	LYS
1	B	73	VAL
1	B	94	ASP
1	B	114	ASN
1	B	137	THR
1	B	139	THR
1	B	141	LYS
1	B	171	GLU
1	B	199	ILE
1	B	239	LEU
1	B	297	ARG
1	B	302	ILE

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Mol	Chain	Res	Type
1	B	314	LYS
1	B	346	PRO
1	B	405	ASN
1	B	471	SER
1	B	474	THR
1	B	537	LYS
1	B	546	LEU
1	B	636	THR
1	B	649	ARG
1	B	683	GLU
1	B	701	ILE
1	B	729	MET
1	B	767	THR
1	C	46	LYS
1	C	57	GLN
1	C	69	LYS
1	C	71	LYS
1	C	92	VAL
1	C	96	ARG
1	C	122	LYS
1	C	139	THR
1	C	141	LYS
1	C	239	LEU
1	C	259	ASN
1	C	297	ARG
1	C	344	VAL
1	C	359	GLN
1	C	364	LYS
1	C	417	TYR
1	C	460	LYS
1	C	472	ASP
1	C	488	LYS
1	C	491	ILE
1	C	546	LEU
1	C	552	ASP
1	C	590	GLN
1	C	595	ARG
1	C	624	LYS
1	C	697	LEU
1	C	729	MET
1	C	751	SER
1	C	767	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	56	GLN
1	A	57	GLN
1	A	66	ASN
1	A	81	GLN
1	A	167	GLN
1	A	238	HIS
1	A	252	HIS
1	A	253	GLN
1	A	415	GLN
1	A	473	HIS
1	A	512	GLN
1	A	598	ASN
1	A	634	ASN
1	A	678	GLN
1	A	738	GLN
1	B	48	HIS
1	B	66	ASN
1	B	167	GLN
1	B	252	HIS
1	B	253	GLN
1	B	259	ASN
1	B	347	HIS
1	B	473	HIS
1	B	590	GLN
1	B	598	ASN
1	B	634	ASN
1	B	738	GLN
1	C	48	HIS
1	C	56	GLN
1	C	57	GLN
1	C	66	ASN
1	C	81	GLN
1	C	167	GLN
1	C	202	HIS
1	C	252	HIS
1	C	253	GLN
1	C	286	GLN
1	C	347	HIS
1	C	359	GLN
1	C	437	ASN

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Mol	Chain	Res	Type
1	C	590	GLN
1	C	634	ASN
1	C	678	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	PCA	B	26	1	7,8,9	2.33	1 (14%)	9,10,12	2.38	5 (55%)
1	PCA	C	26	1	7,8,9	2.41	2 (28%)	9,10,12	2.98	4 (44%)
1	PCA	A	26	1	7,8,9	2.38	1 (14%)	9,10,12	3.38	6 (66%)

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
1	PCA	B	26	1	-	0/0/11/13	0/1/1/1
1	PCA	C	26	1	-	0/0/11/13	0/1/1/1
1	PCA	A	26	1	-	0/0/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	PCA	CD-N	5.99	1.49	1.34
1	C	26	PCA	CD-N	5.84	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	26	PCA	CD-N	5.70	1.48	1.34
1	C	26	PCA	CA-N	2.06	1.48	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	PCA	OE-CD-CG	-5.21	117.42	126.72
1	C	26	PCA	CB-CG-CD	-5.19	96.39	104.41
1	A	26	PCA	CB-CG-CD	-4.93	96.78	104.41
1	A	26	PCA	O-C-CA	-4.73	112.60	124.77
1	C	26	PCA	CB-CA-C	4.50	118.83	112.66
1	B	26	PCA	OE-CD-CG	-4.14	119.34	126.72
1	C	26	PCA	OE-CD-CG	-4.13	119.36	126.72
1	B	26	PCA	O-C-CA	3.44	133.62	124.77
1	A	26	PCA	CG-CB-CA	3.25	117.02	104.33
1	B	26	PCA	CA-N-CD	-2.76	104.12	113.58
1	A	26	PCA	CG-CD-N	2.75	115.12	108.39
1	C	26	PCA	CG-CB-CA	2.74	115.05	104.33
1	B	26	PCA	CB-CA-N	2.61	110.43	103.24
1	A	26	PCA	CB-CA-C	2.45	116.02	112.66
1	B	26	PCA	CG-CD-N	2.43	114.33	108.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	26	PCA	1	0

5.5 Carbohydrates

18 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
2	MAN	D	1	1,2	11,11,12	1.70	2 (18%)	15,15,17	3.16	3 (20%)
2	GCU	D	2	2	12,12,13	1.30	1 (8%)	14,17,19	2.68	3 (21%)
2	XYS	D	3	2	8,8,10	1.56	2 (25%)	8,10,14	2.75	2 (25%)
2	RAM	D	4	2	10,10,11	0.67	0	14,14,16	1.55	1 (7%)
2	MAN	E	1	1,2	11,11,12	1.76	2 (18%)	15,15,17	2.01	4 (26%)
2	GCU	E	2	2	12,12,13	1.30	1 (8%)	14,17,19	2.41	2 (14%)
2	XYS	E	3	2	8,8,10	1.39	1 (12%)	8,10,14	1.28	1 (12%)
2	RAM	E	4	2	10,10,11	0.57	0	14,14,16	0.94	0
2	MAN	F	1	1,2	11,11,12	1.77	2 (18%)	15,15,17	2.84	2 (13%)
2	GCU	F	2	2	12,12,13	1.32	1 (8%)	14,17,19	3.57	3 (21%)
2	XYS	F	3	2	8,8,10	1.54	2 (25%)	8,10,14	3.21	5 (62%)
2	RAM	F	4	2	10,10,11	0.69	0	14,14,16	1.07	0
3	NDG	G	1	3	15,15,15	2.69	2 (13%)	21,21,21	2.95	5 (23%)
3	GCD	G	2	3	10,11,12	2.18	2 (20%)	12,15,17	1.90	4 (33%)
3	NDG	H	1	3	15,15,15	2.88	2 (13%)	21,21,21	2.10	6 (28%)
3	GCD	H	2	3	10,11,12	2.17	2 (20%)	12,15,17	1.64	4 (33%)
3	NDG	I	1	3	15,15,15	2.74	2 (13%)	21,21,21	2.67	9 (42%)
3	GCD	I	2	3	10,11,12	2.35	1 (10%)	12,15,17	1.58	5 (41%)

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
2	MAN	D	1	1,2	-	0/2/19/22	0/1/1/1
2	GCU	D	2	2	-	0/4/21/24	0/1/1/1
2	XYS	D	3	2	-	-	0/1/1/1
2	RAM	D	4	2	-	-	0/1/1/1
2	MAN	E	1	1,2	-	0/2/19/22	0/1/1/1
2	GCU	E	2	2	-	0/4/21/24	0/1/1/1
2	XYS	E	3	2	1/1/2/4	-	0/1/1/1
2	RAM	E	4	2	-	-	0/1/1/1
2	MAN	F	1	1,2	-	2/2/19/22	0/1/1/1
2	GCU	F	2	2	1/1/5/6	1/4/21/24	0/1/1/1
2	XYS	F	3	2	-	-	0/1/1/1
2	RAM	F	4	2	-	-	0/1/1/1
3	NDG	G	1	3	-	2/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GCD	G	2	3	-	4/4/17/20	0/1/1/1
3	NDG	H	1	3	-	1/6/26/26	0/1/1/1
3	GCD	H	2	3	-	0/4/17/20	0/1/1/1
3	NDG	I	1	3	-	3/6/26/26	0/1/1/1
3	GCD	I	2	3	-	2/4/17/20	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1	NDG	O7-C7	10.07	1.45	1.23
3	I	1	NDG	O7-C7	9.56	1.44	1.23
3	G	1	NDG	O7-C7	9.48	1.44	1.23
3	I	2	GCD	O5-C5	6.51	1.46	1.37
3	H	2	GCD	O5-C5	6.07	1.45	1.37
3	G	2	GCD	O5-C5	5.87	1.45	1.37
2	F	1	MAN	O2-C2	-4.21	1.34	1.43
2	E	1	MAN	O2-C2	-4.17	1.34	1.43
3	H	1	NDG	C7-N2	3.97	1.47	1.34
2	D	1	MAN	O2-C2	-3.84	1.35	1.43
2	F	1	MAN	O4-C4	-3.77	1.33	1.43
2	F	2	GCU	O4-C4	-3.60	1.34	1.43
2	D	1	MAN	O4-C4	-3.60	1.34	1.43
3	G	1	NDG	C7-N2	3.50	1.45	1.34
2	E	2	GCU	O4-C4	-3.49	1.34	1.43
2	E	1	MAN	O4-C4	-3.47	1.34	1.43
2	D	2	GCU	O4-C4	-3.42	1.34	1.43
2	E	3	XYS	O5-C1	-3.37	1.36	1.43
3	I	1	NDG	C7-N2	3.31	1.45	1.34
2	F	3	XYS	O5-C1	-3.04	1.37	1.43
2	F	3	XYS	C3-C2	2.93	1.56	1.52
2	D	3	XYS	O5-C1	-2.85	1.37	1.43
2	D	3	XYS	C3-C2	2.75	1.56	1.52
3	G	2	GCD	C5-C6	-2.23	1.43	1.48
3	H	2	GCD	O6B-C6	-2.10	1.24	1.30

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	GCU	O4-C4-C5	12.36	137.99	109.76
2	D	1	MAN	O2-C2-C3	10.55	131.99	110.15
3	G	1	NDG	O7-C7-C8	-9.83	104.56	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	MAN	O2-C2-C3	9.33	129.48	110.15
2	D	2	GCU	O4-C4-C5	8.13	128.34	109.76
2	E	2	GCU	O4-C4-C5	8.03	128.09	109.76
2	F	3	XYS	C4-C3-C2	7.03	116.74	111.12
3	H	1	NDG	O7-C7-C8	-6.66	110.20	122.05
2	D	3	XYS	C4-C3-C2	6.65	116.44	111.12
3	G	1	NDG	C8-C7-N2	-5.81	106.48	116.12
3	I	1	NDG	O7-C7-C8	-5.61	112.07	122.05
3	I	1	NDG	C8-C7-N2	-5.09	107.68	116.12
3	G	1	NDG	C1-C2-C3	4.95	117.30	110.54
2	E	1	MAN	O2-C2-C3	4.71	119.90	110.15
3	I	1	NDG	C2-N2-C7	-4.54	112.48	123.11
2	D	1	MAN	O4-C4-C5	-4.45	98.37	109.32
2	E	1	MAN	O2-C2-C1	4.06	118.52	109.22
2	F	1	MAN	O2-C2-C1	-3.95	100.19	109.22
2	D	4	RAM	C1-O5-C5	3.81	121.94	112.97
3	H	1	NDG	C8-C7-N2	-3.78	109.85	116.12
3	I	1	NDG	O5-C1-C2	3.68	113.21	109.52
2	F	3	XYS	C5-O5-C1	3.67	115.14	110.02
2	D	3	XYS	C5-O5-C1	3.60	115.04	110.02
3	I	1	NDG	O7-C7-N2	3.54	128.23	121.98
2	D	2	GCU	O4-C4-C3	3.45	118.51	110.38
2	D	2	GCU	C1-C2-C3	3.37	114.55	109.64
3	I	1	NDG	C1-C2-C3	3.27	115.01	110.54
3	I	1	NDG	O1-C1-C2	3.26	115.99	109.22
3	H	1	NDG	O7-C7-N2	-3.09	116.53	121.98
2	F	2	GCU	C3-C4-C5	-2.98	104.17	109.30
3	G	2	GCD	C1-C2-C3	2.98	113.98	109.64
3	G	1	NDG	O5-C5-C6	2.97	113.80	106.44
2	F	3	XYS	O5-C5-C4	-2.93	106.69	111.74
3	I	2	GCD	O6B-C6-C5	2.88	120.58	114.06
3	H	2	GCD	O6B-C6-C5	2.83	120.47	114.06
2	E	1	MAN	O3-C3-C2	-2.81	104.31	110.05
3	G	2	GCD	O6A-C6-C5	-2.77	113.77	120.57
2	D	1	MAN	C1-C2-C3	-2.66	105.77	109.64
3	H	2	GCD	O5-C5-C4	-2.65	122.50	124.94
3	H	1	NDG	C1-C2-N2	-2.53	107.80	110.73
3	G	1	NDG	O1-C1-C2	2.48	114.37	109.22
3	I	1	NDG	C1-O5-C5	2.48	118.44	113.65
3	I	1	NDG	C3-C4-C5	-2.45	105.79	110.23
2	E	3	XYS	C4-C3-C2	2.42	113.06	111.12
3	H	2	GCD	C1-C2-C3	2.40	113.14	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	NDG	C2-N2-C7	2.39	128.69	123.11
2	E	1	MAN	C1-C2-C3	-2.33	106.25	109.64
2	F	3	XYS	O3-C3-C4	-2.33	104.30	109.99
3	G	2	GCD	O3-C3-C2	2.26	113.47	109.44
2	F	2	GCU	O4-C4-C3	2.23	115.63	110.38
3	I	2	GCD	O2-C2-C1	2.19	114.23	109.22
2	F	3	XYS	C5-C4-C3	-2.18	107.07	110.61
3	I	2	GCD	C1-C2-C3	2.18	112.81	109.64
2	E	2	GCU	O2-C2-C3	2.12	114.54	110.15
3	I	2	GCD	O5-C5-C6	2.09	115.68	111.85
3	I	2	GCD	O6A-C6-C5	-2.08	115.46	120.57
3	H	1	NDG	O3-C3-C4	2.07	115.27	110.38
3	G	2	GCD	C4-C5-C6	-2.06	119.10	123.56
3	H	2	GCD	O5-C5-C6	2.06	115.63	111.85

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	3	XYS	C1
2	F	2	GCU	C4

All (15) torsion outliers are listed below:

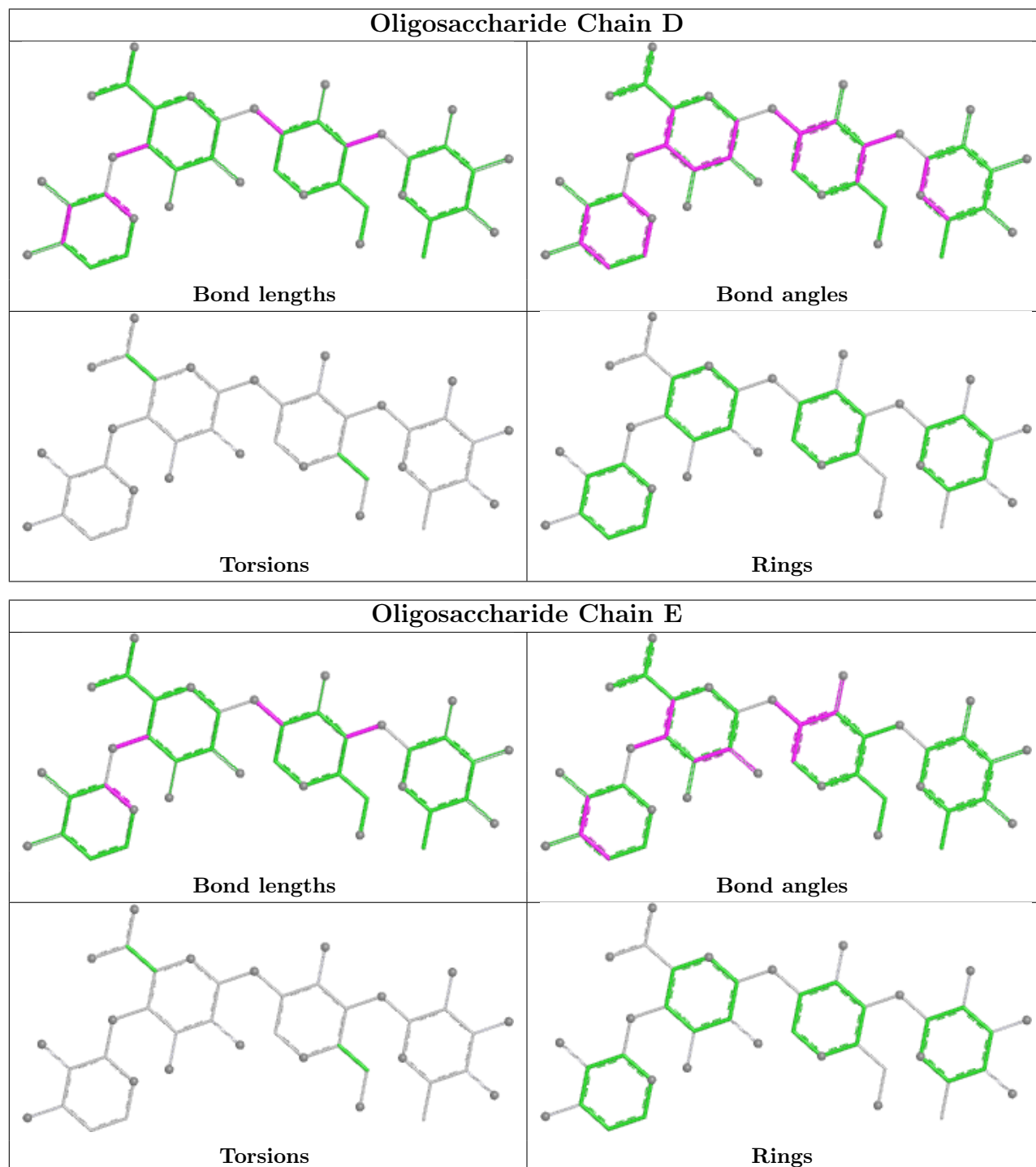
Mol	Chain	Res	Type	Atoms
3	G	2	GCD	O5-C5-C6-O6B
3	G	1	NDG	O7-C7-N2-C2
3	I	1	NDG	C8-C7-N2-C2
3	I	1	NDG	O5-C5-C6-O6
3	H	1	NDG	O7-C7-N2-C2
3	I	1	NDG	C4-C5-C6-O6
3	G	1	NDG	O5-C5-C6-O6
3	G	2	GCD	C4-C5-C6-O6A
3	G	2	GCD	C4-C5-C6-O6B
3	G	2	GCD	O5-C5-C6-O6A
3	I	2	GCD	O5-C5-C6-O6B
2	F	1	MAN	C4-C5-C6-O6
2	F	1	MAN	O5-C5-C6-O6
3	I	2	GCD	O5-C5-C6-O6A
2	F	2	GCU	O5-C5-C6-O6B

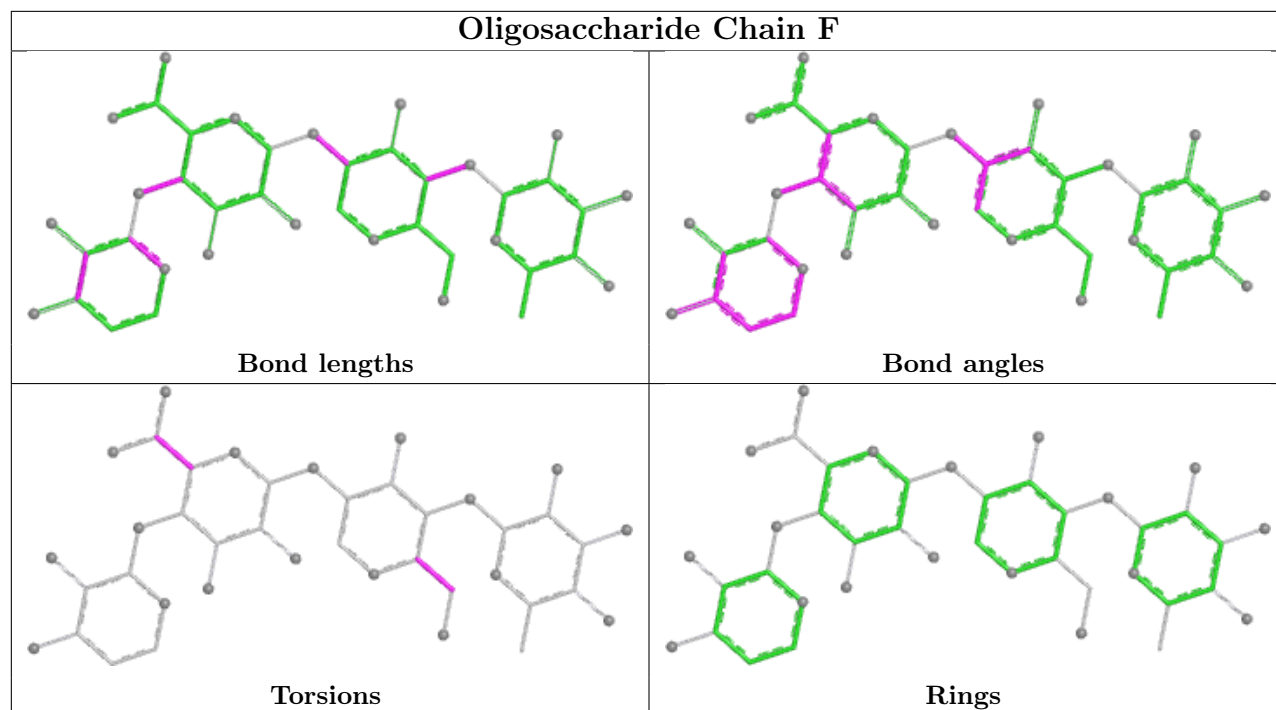
There are no ring outliers.

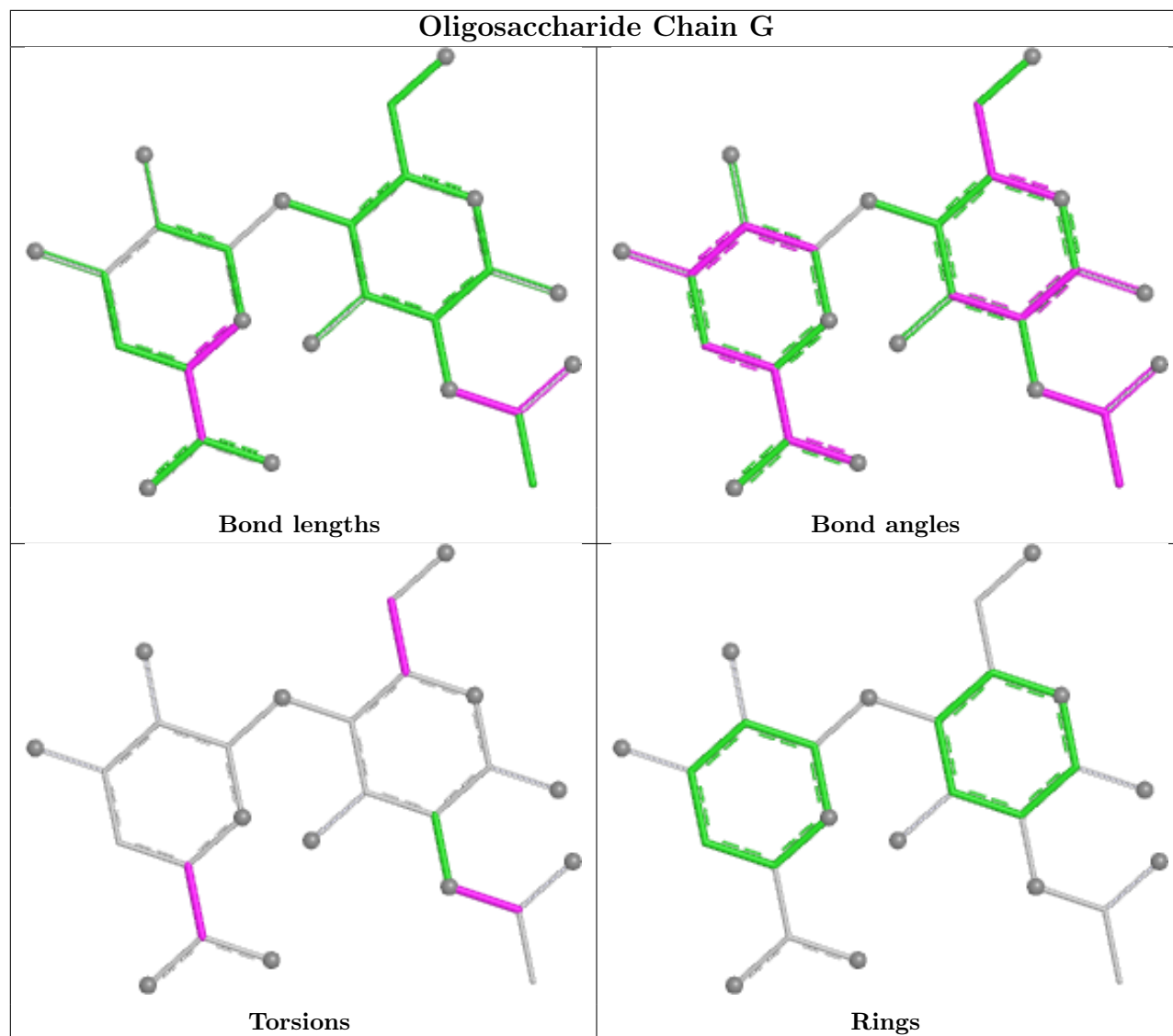
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	NDG	1	0
3	I	2	GCD	2	0
2	E	4	RAM	1	0

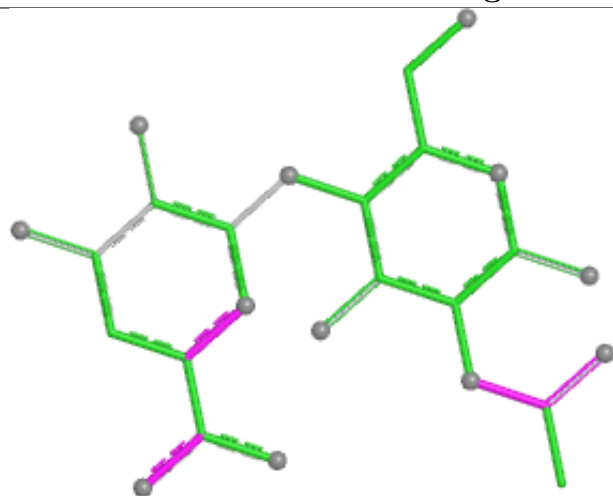
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



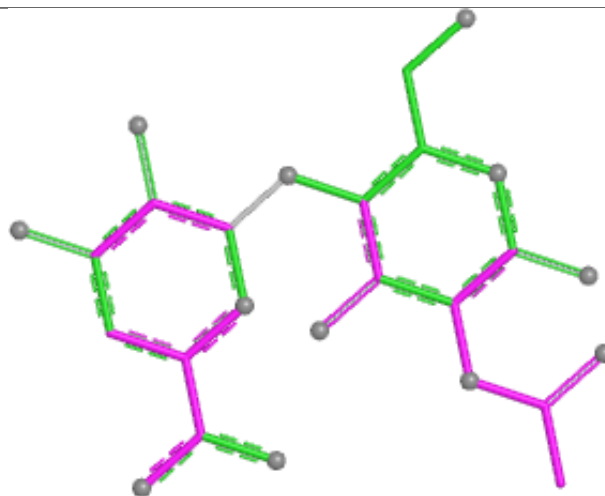




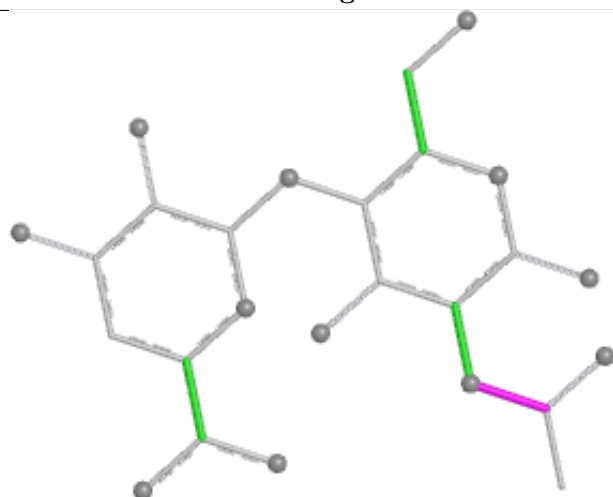
Oligosaccharide Chain H



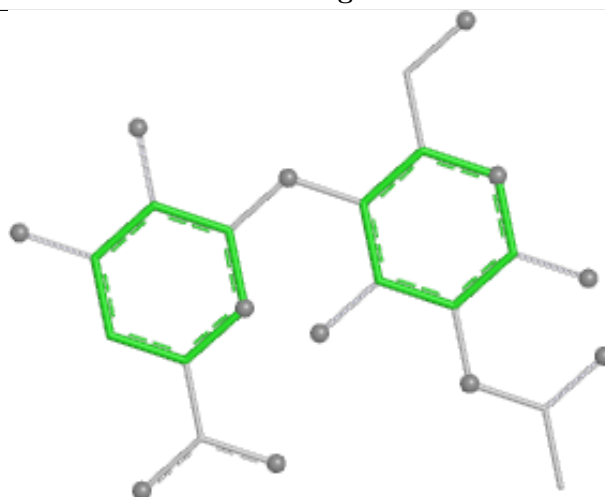
Bond lengths



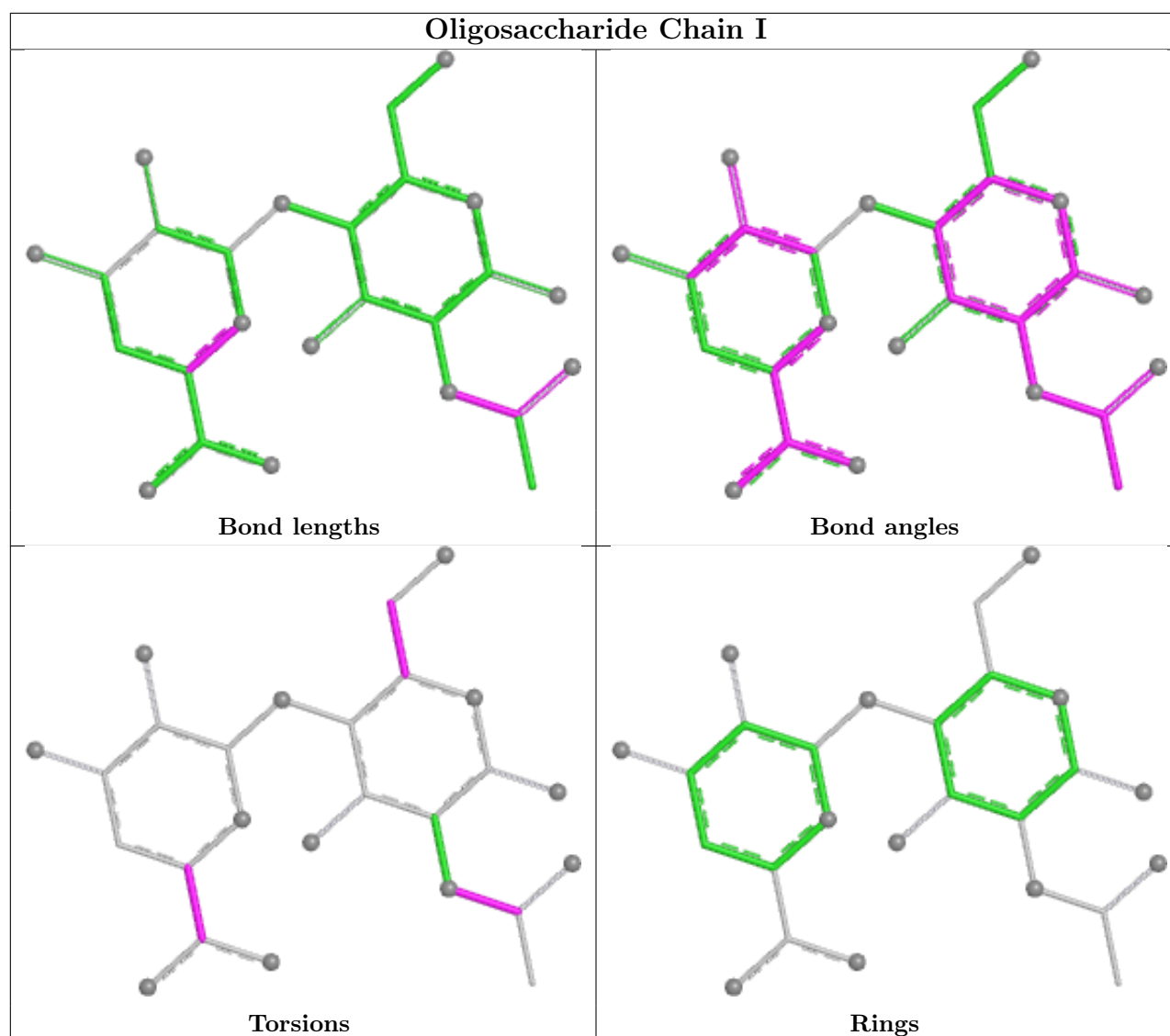
Bond angles



Torsions



Rings



5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 3 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	$\# Z > 2$
5	PO4	A	3	-	4,4,4	0.82	0	6,6,6	0.96	0
5	PO4	A	2	-	4,4,4	0.76	0	6,6,6	1.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PO4	B	1	-	4,4,4	1.07	0	6,6,6	1.69	2 (33%)
5	PO4	B	7	-	4,4,4	0.88	0	6,6,6	0.78	0
5	PO4	B	8	-	4,4,4	0.59	0	6,6,6	0.97	0
5	PO4	C	4	-	4,4,4	0.86	0	6,6,6	1.34	1 (16%)
5	PO4	A	5	-	4,4,4	0.62	0	6,6,6	0.90	0
5	PO4	A	9	-	4,4,4	0.88	0	6,6,6	1.51	1 (16%)
5	PO4	C	6	-	4,4,4	0.49	0	6,6,6	1.71	3 (50%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1	PO4	O4-P-O1	-2.81	101.00	110.95
5	A	9	PO4	O3-P-O2	2.59	115.96	107.91
5	C	6	PO4	O4-P-O3	2.50	115.68	107.91
5	C	4	PO4	O3-P-O2	2.42	115.45	107.91
5	B	1	PO4	O3-P-O1	2.36	119.30	110.95
5	C	6	PO4	O4-P-O1	-2.25	102.99	110.95
5	C	6	PO4	O3-P-O2	2.05	114.28	107.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	6	PO4	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	746/749 (99%)	0.05	0 100 100	19, 24, 27, 31	0
1	B	746/749 (99%)	0.15	6 (0%) 82 86	19, 24, 27, 31	0
1	C	746/749 (99%)	0.16	8 (1%) 78 82	19, 24, 28, 34	0
All	All	2238/2247 (99%)	0.12	14 (0%) 85 89	19, 24, 28, 34	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	471	SER	4.7
1	C	470	GLY	4.6
1	C	472	ASP	4.5
1	C	474	THR	4.0
1	C	473	HIS	3.5
1	B	623	GLY	3.0
1	B	474	THR	2.8
1	C	361	GLY	2.3
1	C	632	GLY	2.3
1	B	629	TRP	2.3
1	B	36	VAL	2.2
1	B	87	ALA	2.2
1	B	39	VAL	2.0
1	C	629	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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($\text{\AA}^2$)	Q<0.9
1	PCA	A	26	8/9	0.75	0.16	28,29,29,31	0
1	PCA	C	26	8/9	0.82	0.13	29,29,30,30	0
1	PCA	B	26	8/9	0.84	0.12	30,31,32,33	0

6.3 Carbohydrates

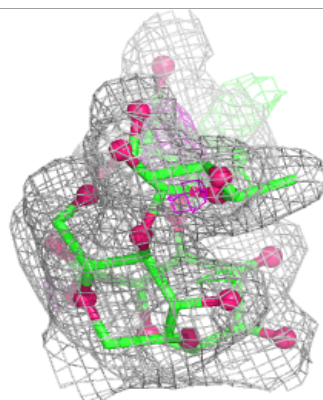
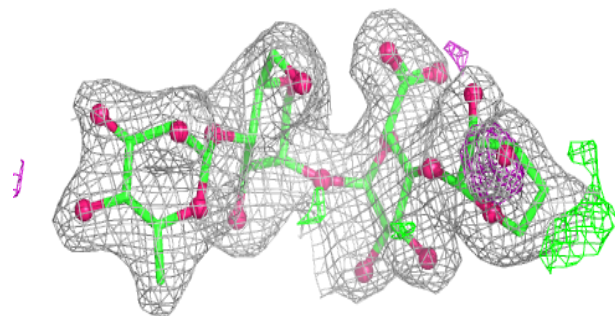
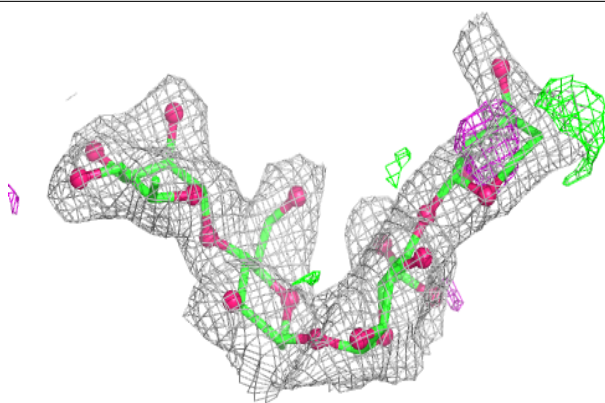
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	XYS	D	3	8/10	0.57	0.19	45,47,47,47	0
2	XYS	F	3	8/10	0.60	0.19	49,49,50,50	0
2	XYS	E	3	8/10	0.67	0.17	48,48,49,49	0
2	GCU	E	2	12/13	0.82	0.11	39,40,42,45	0
3	GCD	I	2	11/12	0.82	0.12	34,34,37,37	0
3	NDG	I	1	15/15	0.86	0.11	32,35,38,38	0
2	GCU	D	2	12/13	0.88	0.08	33,35,36,42	0
2	GCU	F	2	12/13	0.89	0.09	33,35,37,44	0
3	NDG	G	1	15/15	0.90	0.09	26,30,31,33	0
3	GCD	G	2	11/12	0.91	0.09	24,30,31,33	0
2	RAM	E	4	10/11	0.92	0.08	28,29,30,30	0
3	GCD	H	2	11/12	0.93	0.07	21,24,26,27	0
2	MAN	E	1	11/12	0.94	0.07	26,27,29,36	0
3	NDG	H	1	15/15	0.94	0.07	23,26,28,28	0
2	MAN	D	1	11/12	0.94	0.07	24,27,31,35	0
2	RAM	F	4	10/11	0.94	0.07	25,26,28,28	0
2	MAN	F	1	11/12	0.94	0.07	23,27,29,32	0
2	RAM	D	4	10/11	0.95	0.06	23,27,28,30	0

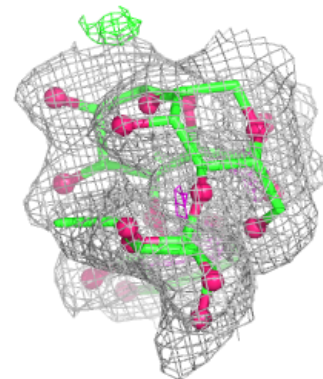
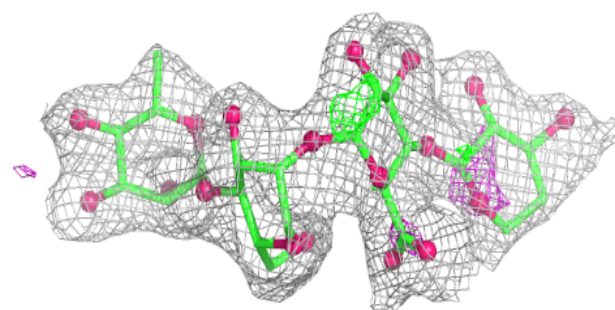
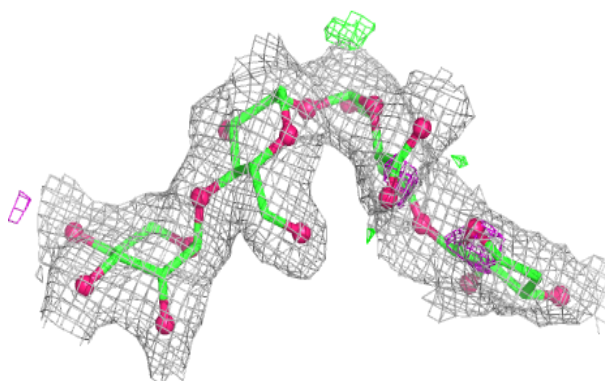
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

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

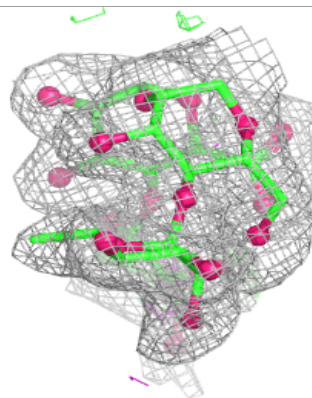
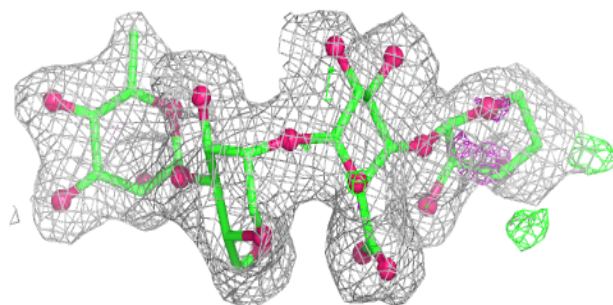
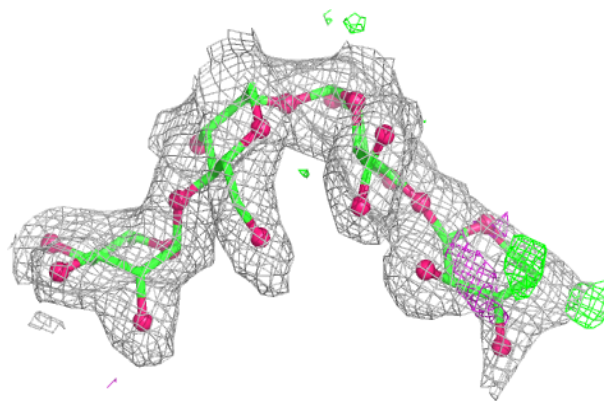
**Electron density around Chain E:**

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



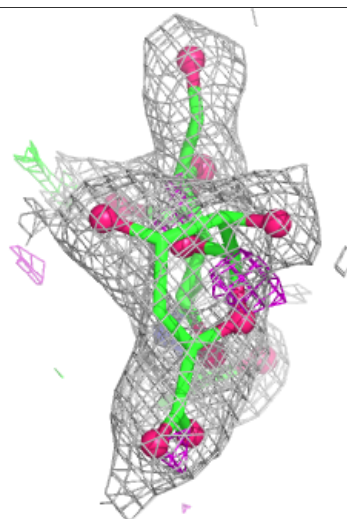
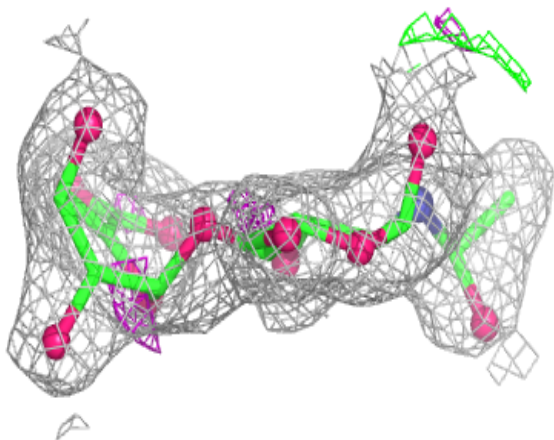
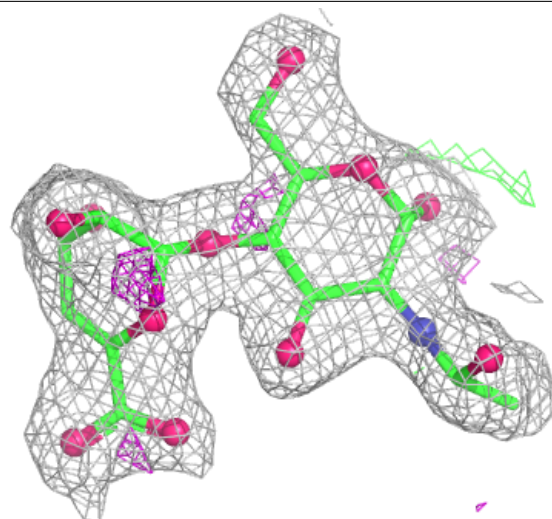
Electron density around Chain F:

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



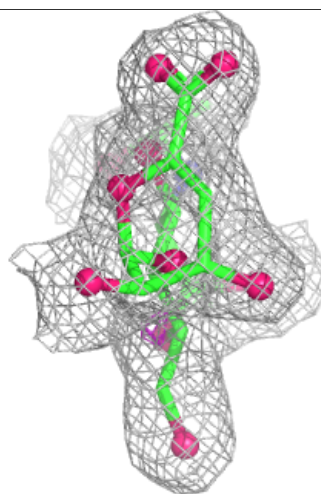
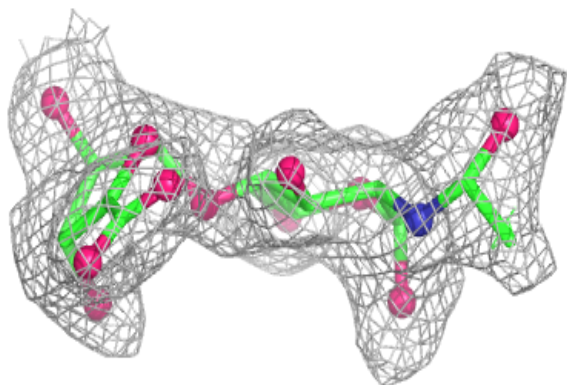
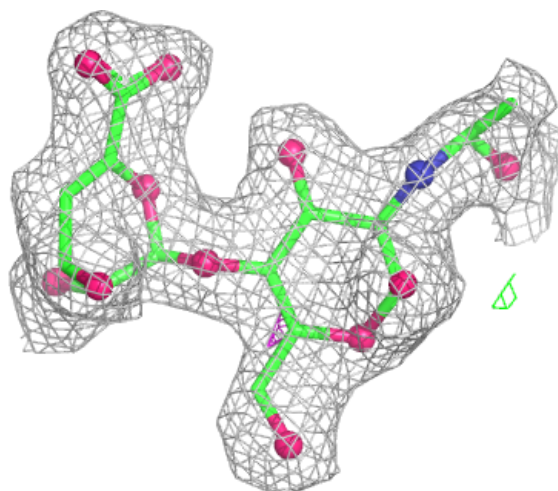
Electron density around Chain G:

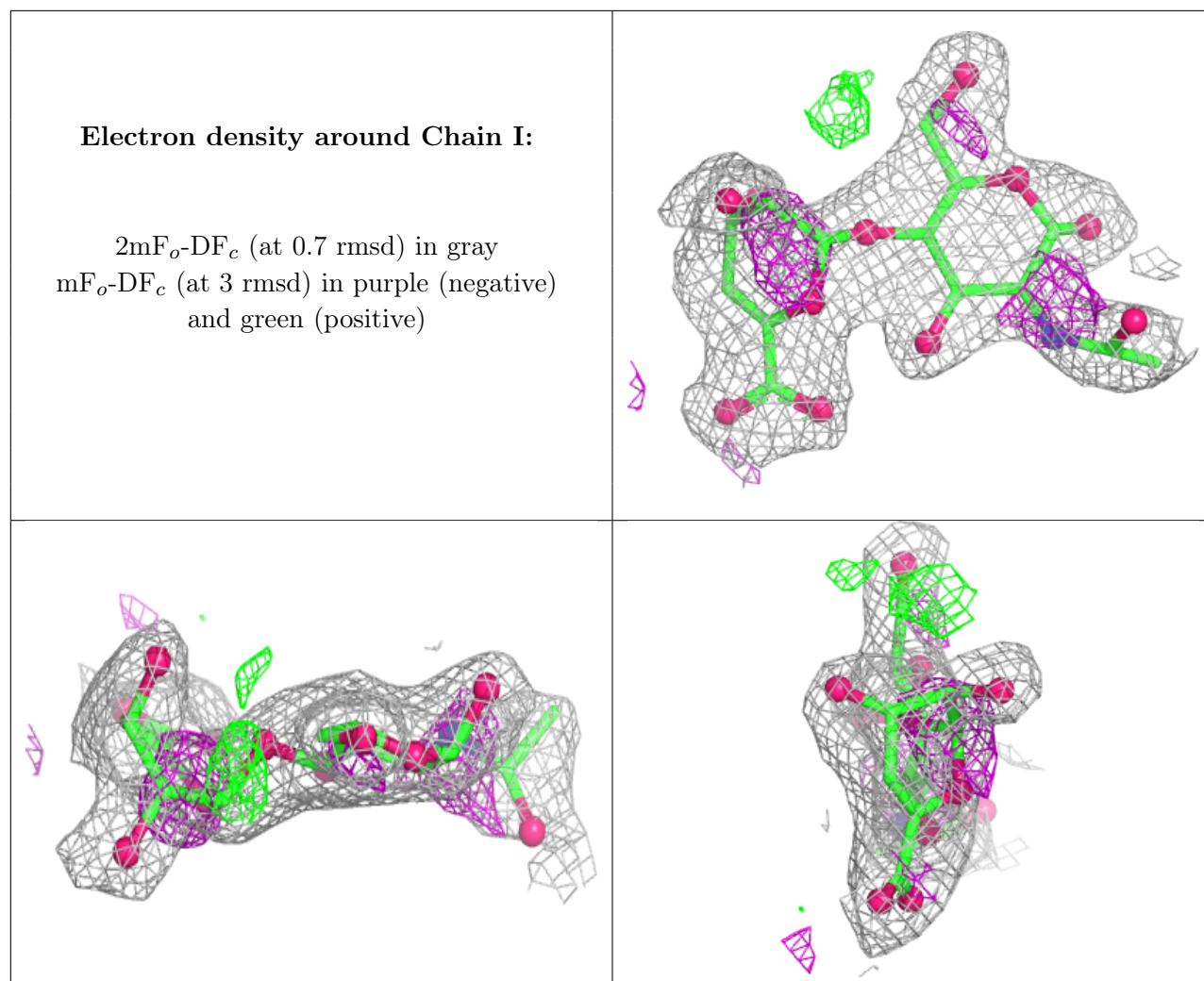
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PO4	C	6	5/5	0.75	0.24	57,57,59,59	0
5	PO4	A	5	5/5	0.84	0.14	52,53,54,54	0
5	PO4	B	8	5/5	0.87	0.17	48,49,49,50	0
5	PO4	B	7	5/5	0.89	0.18	52,52,53,54	0
5	PO4	A	2	5/5	0.90	0.17	44,45,45,45	0
5	PO4	A	3	5/5	0.93	0.14	41,41,42,43	0
5	PO4	C	4	5/5	0.94	0.17	31,31,31,31	0
5	PO4	A	9	5/5	0.97	0.11	26,26,27,27	0
5	PO4	B	1	5/5	0.97	0.12	27,27,28,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ZN	A	1	1/1	1.00	0.09	27,27,27,27	0
4	ZN	B	2	1/1	1.00	0.07	26,26,26,26	0
4	ZN	C	3	1/1	1.00	0.07	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.