Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 07:28 AM JST

PDB ID	:	7F5R
Title	:	Crystal structure of SARS-CoV-2 Y453F-RBD bound to mink ACE2
Authors	:	Wang, X.Q.; Ding, Q.; Lan, J.; Ren, W.L.
Deposited on	:	2021-06-22
Resolution	:	3.01 Å(reported)

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

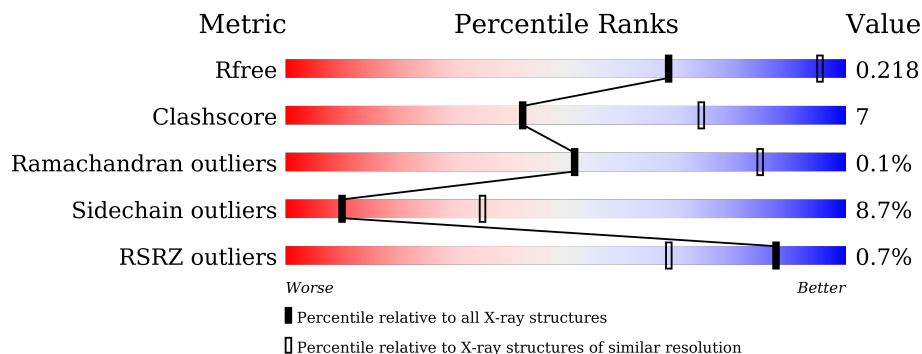|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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.
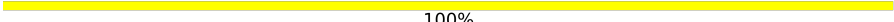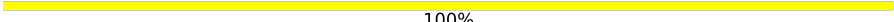
Metric	Percentile Ranks	Value
Rfree		0.218
Clashscore		7
Ramachandran outliers		0.1%
Sidechain outliers		8.7%
RSRZ outliers		0.7%

Worse   Better

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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 <=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	597	78% — 19% — ·
1	B	597	76% — 22% — ·
1	D	597	77% — 20% — ·
2	C	197	78% — 16% — · 5%
2	E	197	70% — 22% — · 6%
2	F	197	81% — 18% — ·

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

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 19386 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 mink ACE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	0	0
			4904	3132	823	920	29			
1	B	596	Total	C	N	O	S	0	0	0
			4904	3132	823	920	29			
1	D	596	Total	C	N	O	S	0	0	0
			4904	3132	823	920	29			

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	185	Total	C	N	O	S	0	0	0
			1468	942	247	271	8			
2	C	187	Total	C	N	O	S	0	0	0
			1483	950	250	275	8			
2	F	197	Total	C	N	O	S	0	0	0
			1559	1000	261	290	8			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	332	PRO	-	expression tag	UNP P0DTC2
E	453	PHE	TYR	variant	UNP P0DTC2
E	528	HIS	-	expression tag	UNP P0DTC2
C	332	PRO	-	expression tag	UNP P0DTC2
C	453	PHE	TYR	variant	UNP P0DTC2
C	528	HIS	-	expression tag	UNP P0DTC2
F	332	PRO	-	expression tag	UNP P0DTC2
F	453	PHE	TYR	variant	UNP P0DTC2
F	528	HIS	-	expression tag	UNP P0DTC2

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.
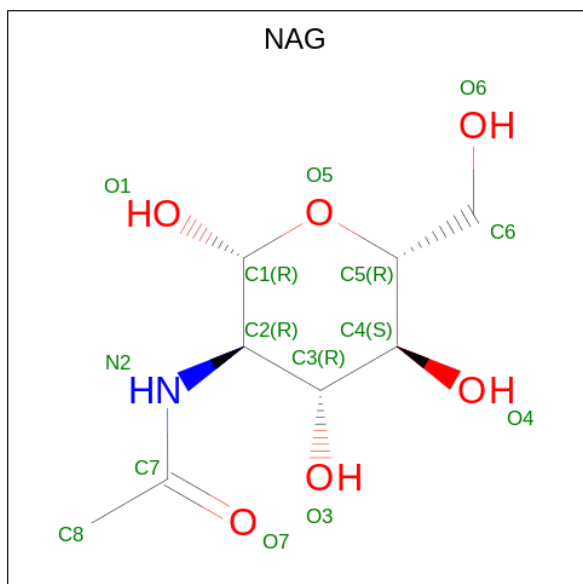
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	2	Total 28	C 16	N 2	O 10	0	0	0
3	I	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 4 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	2	Total 24	C 14	N 1	O 9	0	0	0

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

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

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

3 Residue-property plots ⓘ

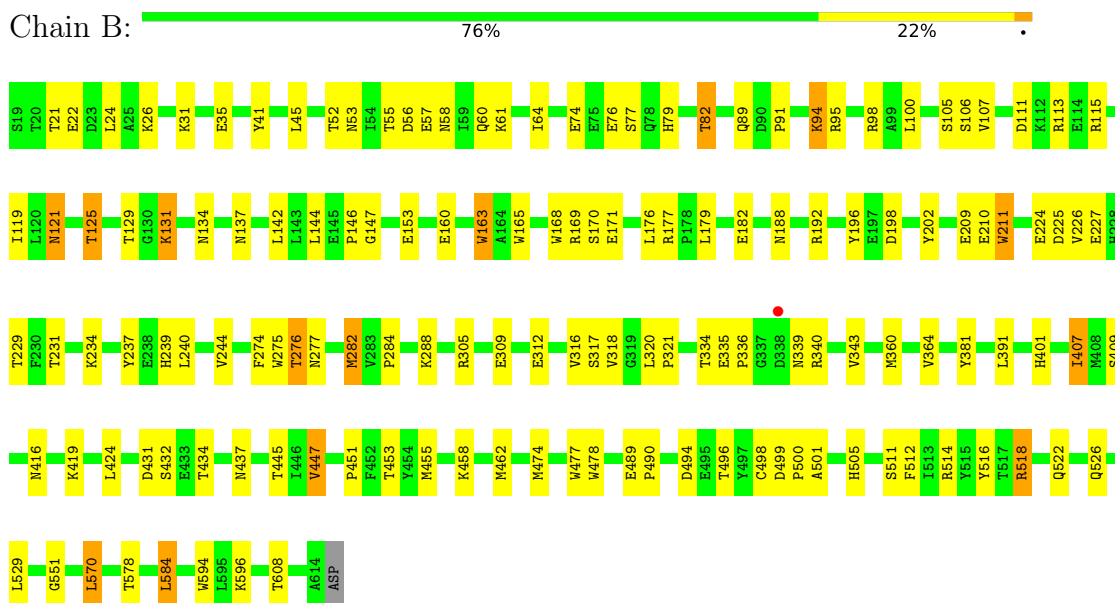These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: mink ACE2
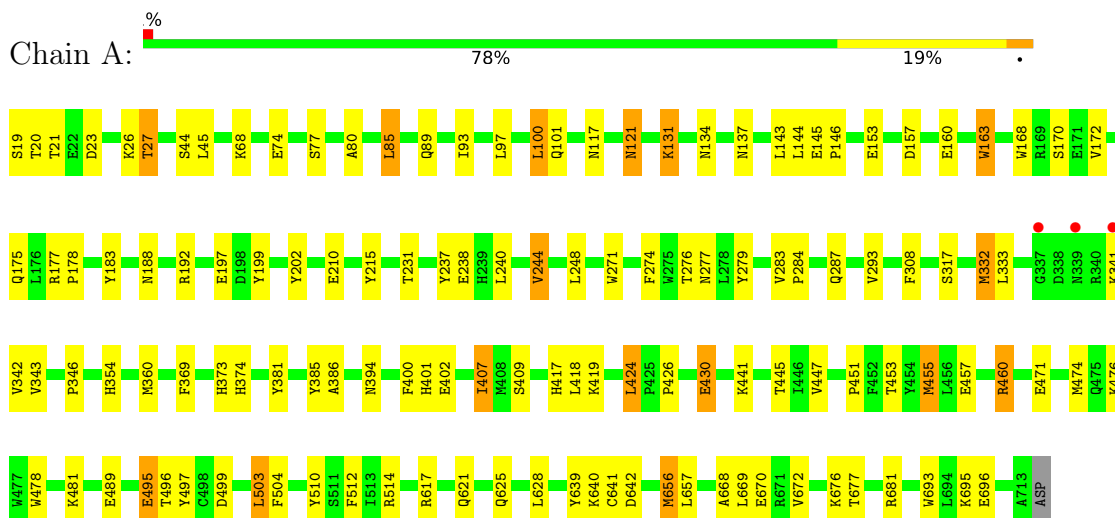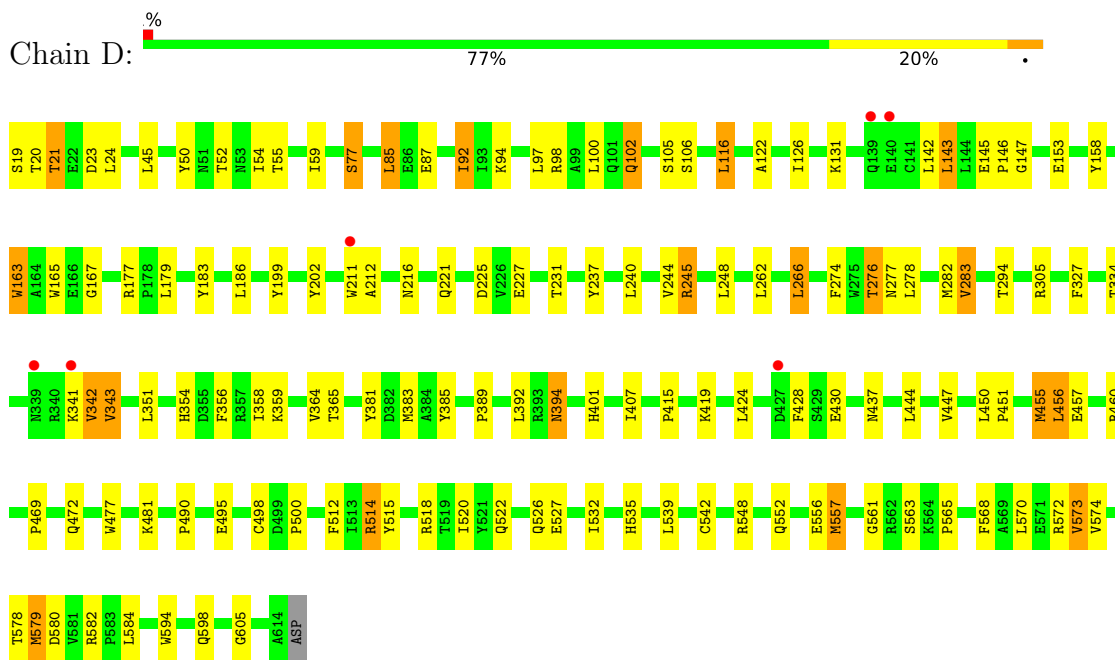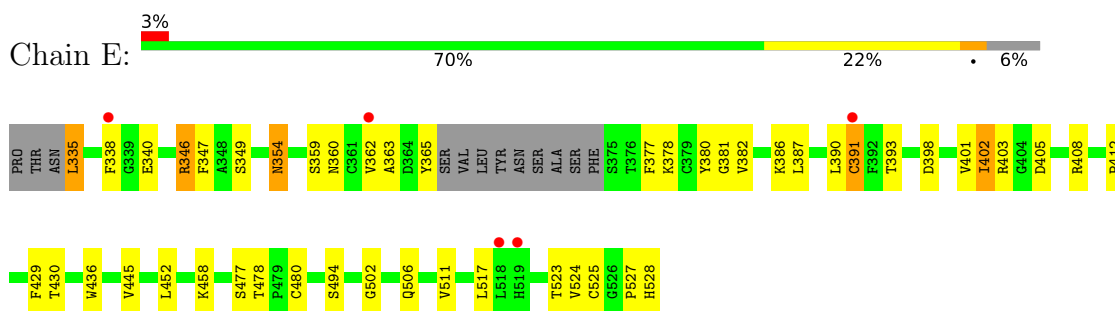
• Molecule 1: mink ACE2

• Molecule 1: mink ACE2

Chain D:

Chain D residue bars (S19–ASP614)

• Molecule 2: Spike protein S1

Chain E:

Chain E residue bars (PRO–H528)

• Molecule 2: Spike protein S1

Chain C:

Chain C residue bars (PRO–H528)

• Molecule 2: Spike protein S1

Chain F:

Chain F residue bars (P332–H528)
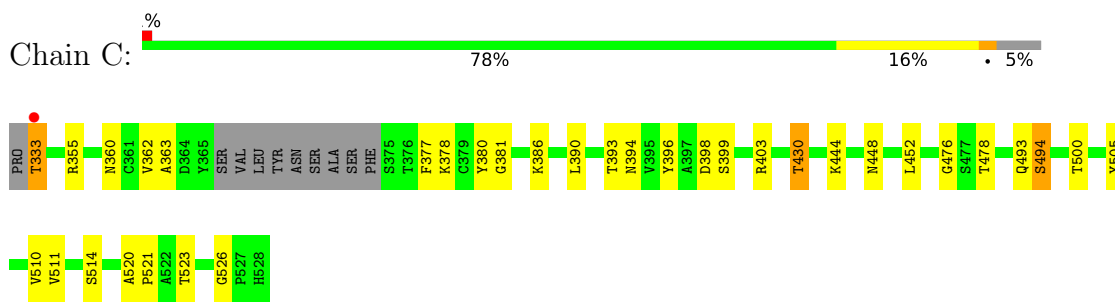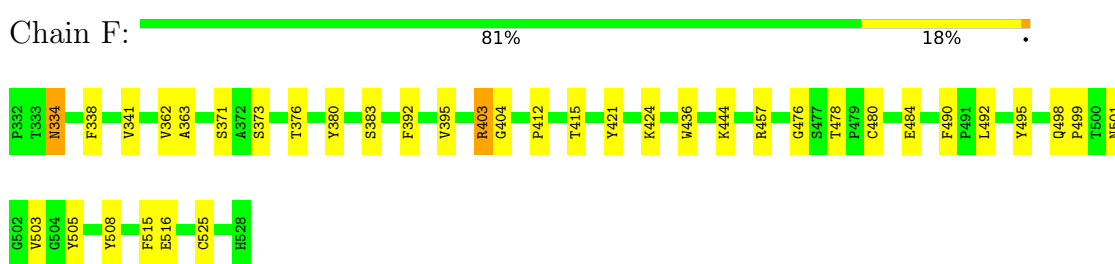
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc
opyranose

Chain G:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc
opyranose

Chain I:

• Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	290.19Å 130.19Å 136.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.53 – 3.01 43.53 – 3.01	Depositor EDS
% Data completeness (in resolution range)	98.1 (43.53-3.01) 98.1 (43.53-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.181 , 0.218 0.181 , 0.218	Depositor DCC
R_{free} test set	5072 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	68.6	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 31.8	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19386	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality (i)

5.1   Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, 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	0.52	3/5047 (0.1%)	0.62	0/6855
1	B	0.49	0/5047	0.63	3/6855 (0.0%)
1	D	0.47	0/5047	0.62	2/6855 (0.0%)
2	C	0.51	0/1525	0.66	0/2074
2	E	0.53	0/1510	0.68	1/2053 (0.0%)
2	F	0.57	1/1605 (0.1%)	0.67	0/2185
All	All	0.50	4/19781 (0.0%)	0.63	6/26877 (0.0%)

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	B	0	1
1	D	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	74	GLU	CG-CD	6.36	1.61	1.51
1	A	74	GLU	CB-CG	6.29	1.64	1.52
1	A	74	GLU	CD-OE1	5.48	1.31	1.25
2	F	484	GLU	CG-CD	5.36	1.59	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	584	LEU	CA-CB-CG	7.66	132.92	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	456	LEU	CA-CB-CG	6.94	131.27	115.30
1	B	169	ARG	NE-CZ-NH1	-6.48	117.06	120.30
1	D	584	LEU	CA-CB-CG	6.00	129.09	115.30
2	E	380	TYR	C-N-CA	-5.87	109.98	122.30
1	B	98	ARG	NE-CZ-NH2	-5.51	117.55	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	52	THR	Peptide
1	D	102	GLN	Peptide

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	4904	0	4657	65	0
1	B	4904	0	4656	71	0
1	D	4904	0	4658	77	0
2	C	1483	0	1402	18	0
2	E	1468	0	1390	18	0
2	F	1559	0	1475	16	0
3	G	28	0	25	0	0
3	I	28	0	25	0	0
4	H	24	0	22	0	0
5	A	14	0	13	0	0
5	B	42	0	39	1	0
5	D	14	0	13	0	0
5	E	14	0	13	0	0
All	All	19386	0	18388	261	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 7.

All (261) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:GLU:OE1	1:A:460:ARG:NH1	1.95	0.98
1:B:288:LYS:HB3	1:B:434:THR:HG22	1.50	0.93
2:E:346:ARG:NH1	2:E:347:PHE:O	2.13	0.81
1:A:192:ARG:NH1	1:A:197:GLU:O	2.18	0.77
1:A:23:ASP:O	1:A:27:THR:HG22	1.85	0.76
1:B:53:ASN:HB3	1:B:340:ARG:HG2	1.68	0.76
2:E:381:GLY:HA3	2:E:430:THR:HG23	1.69	0.74
1:B:55:THR:HG22	1:B:58:ASN:H	1.54	0.73
1:A:271:TRP:CE2	1:A:503:LEU:HD23	2.24	0.72
1:B:229:THR:HG23	1:B:516:TYR:OH	1.90	0.72
1:B:340:ARG:HD2	5:B:904:NAG:H82	1.74	0.70
1:D:573:VAL:HG23	1:D:574:VAL:HG13	1.73	0.70
1:A:474:MET:N	1:A:495:GLU:OE1	2.25	0.69
1:D:177:ARG:NH1	1:D:495:GLU:O	2.26	0.69
1:A:419:LYS:NZ	1:A:426:PRO:O	2.28	0.67
1:D:245:ARG:HH11	1:D:245:ARG:HG2	1.60	0.66
1:D:294:THR:HG23	1:D:365:THR:HA	1.78	0.65
1:A:460:ARG:NH2	1:A:510:TYR:O	2.29	0.65
2:E:335:LEU:HB2	2:E:362:VAL:HG12	1.79	0.65
1:B:94:LYS:HE3	1:B:211:TRP:CD1	2.32	0.64
1:A:400:PHE:HE2	1:A:656:MET:HE1	1.63	0.64
2:E:360:ASN:HA	2:E:523:THR:HB	1.81	0.63
1:A:77:SER:OG	1:A:100:LEU:O	2.16	0.62
2:F:334:ASN:OD1	2:F:334:ASN:N	2.33	0.62
2:E:403:ARG:NH1	2:E:405:ASP:OD2	2.32	0.62
2:F:490:PHE:HE1	2:F:492:LEU:HB2	1.66	0.60
1:B:477:TRP:CE3	1:B:500:PRO:HG3	2.36	0.60
1:B:407:ILE:HD11	1:B:526:GLN:HB2	1.85	0.59
1:B:458:LYS:HE2	1:B:462:MET:HE2	1.85	0.59
1:D:142:LEU:HD22	1:D:147:GLY:HA3	1.85	0.59
1:A:455:MET:HE1	1:A:481:LYS:HE2	1.84	0.59
1:A:131:LYS:HB3	1:A:143:LEU:HD23	1.86	0.58
1:A:274:PHE:HB3	1:A:276:THR:HG22	1.85	0.58
1:D:274:PHE:HB3	1:D:276:THR:HG23	1.86	0.58
1:D:343:VAL:O	1:D:359:LYS:HE2	2.04	0.58
1:B:274:PHE:HB3	1:B:276:THR:HG22	1.85	0.58
1:D:455:MET:HE1	1:D:481:LYS:HE2	1.86	0.57
1:A:157:ASP:HB3	1:A:160:GLU:HB3	1.86	0.57
1:A:97:LEU:O	1:A:101:GLN:HG2	2.04	0.57
1:B:77:SER:HB2	1:B:100:LEU:O	2.04	0.57
1:A:80:ALA:HB2	1:A:100:LEU:HD13	1.87	0.57
1:D:212:ALA:O	1:D:216:ASN:ND2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:PRO:HG2	1:D:392:LEU:HD12	1.86	0.57
1:D:457:GLU:OE1	1:D:460:ARG:NH1	2.33	0.57
2:C:363:ALA:O	2:C:526:GLY:HA2	2.05	0.57
1:D:77:SER:OG	1:D:100:LEU:O	2.23	0.56
1:A:346:PRO:HB3	1:A:360:MET:HG3	1.87	0.56
1:B:225:ASP:O	1:B:229:THR:HG22	2.06	0.55
2:C:355:ARG:HD3	2:C:396:TYR:HD2	1.72	0.55
1:A:276:THR:HB	1:A:445:THR:OG1	2.06	0.55
1:B:318:VAL:O	1:B:551:GLY:HA3	2.06	0.55
1:A:240:LEU:O	1:A:244:VAL:HG13	2.07	0.55
1:A:168:TRP:CZ3	1:A:172:VAL:HG21	2.41	0.55
1:D:245:ARG:HB2	1:D:262:LEU:HD21	1.88	0.55
1:D:145:GLU:HB3	1:D:146:PRO:HD3	1.88	0.55
1:B:129:THR:O	1:B:131:LYS:NZ	2.40	0.54
2:C:333:THR:HG22	2:C:362:VAL:HG21	1.88	0.54
2:F:362:VAL:HA	2:F:525:CYS:O	2.08	0.54
1:D:514:ARG:HG2	1:D:515:TYR:N	2.21	0.54
1:B:55:THR:HB	1:B:58:ASN:HB2	1.90	0.54
1:B:153:GLU:HG2	1:B:277:ASN:ND2	2.23	0.54
1:B:79:HIS:O	1:B:82:THR:HG23	2.09	0.53
1:D:407:ILE:HD11	1:D:522:GLN:O	2.07	0.53
2:E:452:LEU:HD23	2:E:494:SER:HA	1.91	0.53
1:D:535:HIS:CE1	1:D:542:CYS:HA	2.44	0.53
1:B:121:ASN:O	1:B:125:THR:HG23	2.08	0.53
1:B:210:GLU:HB3	1:B:211:TRP:CE3	2.43	0.53
1:D:21:THR:HG21	1:D:87:GLU:OE2	2.09	0.53
1:A:144:LEU:HB2	1:A:168:TRP:CZ3	2.45	0.52
1:A:407:ILE:HD11	1:A:621:GLN:O	2.09	0.52
2:C:444:LYS:HG3	2:C:448:ASN:HB2	1.90	0.52
1:D:163:TRP:CD1	1:D:163:TRP:C	2.83	0.52
1:A:354:HIS:HB2	2:E:502:GLY:HA3	1.92	0.52
1:B:284:PRO:HB3	1:B:594:TRP:CZ2	2.45	0.52
1:D:50:TYR:CE1	1:D:54:ILE:HG23	2.45	0.51
1:D:227:GLU:O	1:D:231:THR:HG23	2.10	0.51
1:D:240:LEU:HD22	1:D:447:VAL:HG22	1.90	0.51
1:A:284:PRO:HB3	1:A:693:TRP:CH2	2.46	0.51
2:C:380:TYR:O	2:C:430:THR:HA	2.11	0.51
2:C:381:GLY:HA3	2:C:430:THR:HG22	1.93	0.51
1:D:548:ARG:O	1:D:552:GLN:HG2	2.11	0.51
1:A:215:TYR:OH	1:A:670:GLU:OE1	2.17	0.51
1:B:237:TYR:CD1	1:B:451:PRO:HG2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:THR:HA	1:D:342:VAL:HG22	1.93	0.51
1:D:477:TRP:CZ3	1:D:500:PRO:HB3	2.46	0.51
2:C:360:ASN:HA	2:C:523:THR:HB	1.92	0.50
2:E:338:PHE:HE2	2:E:363:ALA:HB1	1.76	0.50
1:D:20:THR:HG23	1:D:23:ASP:H	1.76	0.50
1:B:22:GLU:OE1	1:B:89:GLN:HG3	2.11	0.50
1:B:177:ARG:HB2	1:B:498:CYS:HB2	1.94	0.50
2:F:403:ARG:HD3	2:F:505:TYR:HA	1.93	0.50
1:A:400:PHE:CE2	1:A:656:MET:HE1	2.45	0.50
1:A:163:TRP:CD1	1:A:163:TRP:C	2.85	0.50
1:B:24:LEU:HD21	2:C:476:GLY:HA2	1.94	0.50
1:A:85:LEU:HD22	1:A:101:GLN:OE1	2.12	0.50
1:B:160:GLU:HG3	1:B:163:TRP:HZ3	1.76	0.50
1:B:511:SER:O	1:B:514:ARG:NH1	2.45	0.50
1:D:158:TYR:CD2	1:D:266:LEU:HD21	2.47	0.50
1:B:474:MET:HE1	1:B:499:ASP:HB2	1.94	0.49
2:F:444:LYS:O	2:F:499:PRO:HD3	2.12	0.49
2:F:490:PHE:CE1	2:F:492:LEU:HB2	2.46	0.49
2:F:498:GLN:H	2:F:501:ASN:ND2	2.09	0.49
1:D:274:PHE:HB3	1:D:276:THR:CG2	2.43	0.49
1:D:245:ARG:NH2	1:D:605:GLY:O	2.45	0.49
1:A:407:ILE:HD12	1:A:625:GLN:HB2	1.95	0.49
1:B:237:TYR:CE1	1:B:451:PRO:HG2	2.48	0.49
1:A:453:THR:HG23	1:A:512:PHE:CD2	2.48	0.49
1:B:477:TRP:CZ3	1:B:500:PRO:HG3	2.49	0.48
1:A:402:GLU:HG3	1:A:617:ARG:NH1	2.28	0.48
1:B:312:GLU:O	1:B:316:VAL:HG23	2.13	0.48
1:D:283:VAL:HG23	1:D:437:ASN:ND2	2.28	0.48
1:A:656:MET:CE	1:A:668:ALA:HB1	2.43	0.48
1:B:514:ARG:O	1:B:518:ARG:HG2	2.14	0.48
2:C:394:ASN:HB3	2:C:396:TYR:CE1	2.48	0.48
1:B:91:PRO:O	1:B:95:ARG:HG2	2.14	0.48
1:D:356:PHE:CE2	1:D:383:MET:HG2	2.49	0.48
1:D:237:TYR:CE1	1:D:451:PRO:HG2	2.48	0.48
1:A:457:GLU:HG2	1:A:512:PHE:HB3	1.96	0.48
1:B:53:ASN:OD1	1:B:53:ASN:N	2.46	0.48
1:D:469:PRO:HG2	1:D:472:GLN:HG2	1.96	0.48
2:C:520:ALA:HB1	2:C:521:PRO:HD2	1.95	0.48
1:D:327:PHE:HE2	1:D:358:ILE:HG13	1.79	0.47
2:F:395:VAL:HG22	2:F:515:PHE:HD1	1.79	0.47
2:E:412:PRO:HG3	2:E:429:PHE:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:LYS:O	1:B:64:ILE:HG13	2.14	0.47
1:A:374:HIS:HE1	1:A:402:GLU:OE2	1.98	0.47
1:A:474:MET:HB3	1:A:474:MET:HE3	1.77	0.47
1:A:656:MET:HG3	1:A:657:LEU:N	2.29	0.47
2:E:527:PRO:O	2:E:528:HIS:HB2	2.15	0.47
1:D:237:TYR:CD1	1:D:451:PRO:HG2	2.50	0.47
1:B:188:ASN:O	1:B:192:ARG:HG3	2.15	0.47
1:B:320:LEU:HB3	1:B:321:PRO:HD2	1.97	0.47
1:A:188:ASN:O	1:A:192:ARG:HG3	2.15	0.47
1:A:20:THR:O	1:A:23:ASP:HB2	2.15	0.46
1:B:407:ILE:CD1	1:B:526:GLN:HB2	2.44	0.46
1:D:116:LEU:HB2	1:D:186:LEU:HD13	1.98	0.46
1:A:134:ASN:HD22	1:A:137:ASN:HB3	1.79	0.46
1:A:639:TYR:O	1:A:640:LYS:HB2	2.15	0.46
1:D:199:TYR:O	1:D:202:TYR:HB3	2.16	0.46
1:B:115:ARG:NH1	1:B:182:GLU:OE2	2.49	0.46
1:D:142:LEU:HD23	1:D:142:LEU:HA	1.81	0.46
1:A:489:GLU:O	1:A:489:GLU:HG2	2.16	0.46
1:D:248:LEU:HD23	1:D:248:LEU:HA	1.80	0.46
1:A:656:MET:HG2	1:A:672:VAL:HG21	1.98	0.46
2:C:399:SER:HA	2:C:510:VAL:O	2.16	0.46
1:D:122:ALA:O	1:D:126:ILE:HG23	2.16	0.46
1:B:94:LYS:HE3	1:B:211:TRP:NE1	2.31	0.45
2:C:403:ARG:HD2	2:C:505:TYR:HA	1.97	0.45
1:D:282:MET:HE1	1:D:444:LEU:HD21	1.97	0.45
1:A:369:PHE:CE1	1:A:373:HIS:HE1	2.35	0.45
1:D:245:ARG:HG2	1:D:245:ARG:NH1	2.31	0.45
1:A:175:GLN:O	1:A:178:PRO:HD2	2.16	0.45
1:B:31:LYS:HE3	1:B:35:GLU:OE2	2.17	0.45
1:D:131:LYS:HE3	1:D:143:LEU:HD13	1.98	0.45
1:A:293:VAL:HG11	1:A:418:LEU:HD22	1.99	0.45
1:D:527:GLU:HG3	1:D:539:LEU:HD22	1.99	0.45
1:B:239:HIS:CE1	1:B:596:LYS:HG2	2.52	0.44
1:B:163:TRP:CD1	1:B:163:TRP:C	2.90	0.44
1:A:424:LEU:HD12	1:A:424:LEU:HA	1.78	0.44
1:B:41:TYR:CE2	1:B:45:LEU:HD22	2.52	0.44
1:B:305:ARG:O	1:B:309:GLU:HG3	2.16	0.44
1:A:354:HIS:CE1	1:A:386:ALA:HB1	2.52	0.44
2:E:391:CYS:HA	2:E:524:VAL:O	2.17	0.44
2:E:402:ILE:HD12	2:E:402:ILE:HA	1.55	0.44
1:B:95:ARG:NH1	1:B:209:GLU:OE2	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:THR:HB	1:B:445:THR:OG1	2.17	0.44
2:C:386:LYS:HB3	2:C:386:LYS:HE3	1.86	0.44
1:A:503:LEU:HD22	1:A:504:PHE:H	1.82	0.44
1:D:447:VAL:HA	1:D:450:LEU:HD12	2.00	0.44
2:F:380:TYR:CE2	2:F:412:PRO:HD2	2.53	0.44
2:C:390:LEU:HD23	2:C:390:LEU:HA	1.77	0.44
1:D:594:TRP:CH2	1:D:598:GLN:HG3	2.52	0.44
1:A:26:LYS:HB2	1:A:93:ILE:HD11	1.99	0.43
1:B:240:LEU:HD22	1:B:447:VAL:CG2	2.48	0.43
1:B:391:LEU:HD23	1:B:391:LEU:HA	1.78	0.43
1:D:240:LEU:O	1:D:244:VAL:HG12	2.18	0.43
2:F:371:SER:HG	2:F:373:SER:HG	1.65	0.43
2:F:421:TYR:CD1	2:F:457:ARG:HB3	2.53	0.43
2:C:452:LEU:HD23	2:C:494:SER:HA	1.99	0.43
1:D:419:LYS:HE3	1:D:428:PHE:HB3	2.00	0.43
2:F:392:PHE:CD1	2:F:515:PHE:HB3	2.53	0.43
1:B:142:LEU:HB3	1:B:147:GLY:HA3	2.01	0.43
1:B:196:TYR:CD2	1:B:202:TYR:HA	2.53	0.43
1:B:416:ASN:O	1:B:419:LYS:HB2	2.19	0.43
1:D:98:ARG:HH21	1:D:211:TRP:HZ2	1.66	0.43
1:D:514:ARG:O	1:D:518:ARG:HG2	2.17	0.43
1:A:471:GLU:CD	1:A:471:GLU:H	2.21	0.43
1:D:50:TYR:HE1	1:D:54:ILE:HG23	1.83	0.43
1:D:177:ARG:HB2	1:D:498:CYS:HB2	1.99	0.43
1:D:565:PRO:O	1:D:568:PHE:N	2.51	0.43
1:B:494:ASP:OD1	1:B:496:THR:HG22	2.18	0.43
2:F:516:GLU:HG3	2:F:516:GLU:O	2.18	0.43
2:E:378:LYS:HA	2:C:378:LYS:HA	2.00	0.43
1:B:431:ASP:HB3	1:B:434:THR:HG23	2.01	0.43
1:D:92:ILE:HA	1:D:92:ILE:HD12	1.79	0.43
1:D:457:GLU:HG2	1:D:512:PHE:HB3	2.01	0.43
1:A:308:PHE:CD1	1:A:333:LEU:HD13	2.53	0.43
1:D:179:LEU:HD23	1:D:179:LEU:HA	1.83	0.43
1:D:351:LEU:HD12	1:D:351:LEU:H	1.84	0.43
1:A:244:VAL:HG23	1:A:248:LEU:HD12	2.01	0.43
1:A:430:GLU:OE2	1:A:640:LYS:HD3	2.19	0.43
1:D:97:LEU:HD23	1:D:97:LEU:HA	1.74	0.43
1:D:165:TRP:CH2	1:D:490:PRO:HD2	2.54	0.43
1:A:474:MET:HE1	1:A:499:ASP:HB2	1.99	0.43
1:D:580:ASP:OD1	1:D:582:ARG:HG3	2.18	0.43
2:E:401:VAL:HG23	2:E:402:ILE:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:398:ASP:O	2:E:511:VAL:HA	2.19	0.42
1:B:570:LEU:HD23	1:B:570:LEU:HA	1.81	0.42
1:A:199:TYR:O	1:A:202:TYR:HB3	2.20	0.42
1:B:165:TRP:CH2	1:B:490:PRO:HD2	2.54	0.42
1:B:244:VAL:HG11	1:B:275:TRP:CZ3	2.54	0.42
1:D:145:GLU:OE1	1:D:145:GLU:HA	2.20	0.42
1:D:579:MET:HE2	1:D:579:MET:HB2	1.83	0.42
1:A:237:TYR:CD1	1:A:451:PRO:HG2	2.54	0.42
1:B:505:HIS:ND1	1:B:505:HIS:N	2.67	0.42
1:B:105:SER:HB3	1:B:113:ARG:HG3	2.02	0.42
1:B:55:THR:HG22	1:B:57:GLU:N	2.35	0.42
1:D:407:ILE:HD12	1:D:526:GLN:HB2	2.02	0.42
1:A:478:TRP:CE3	1:A:489:GLU:HB3	2.55	0.42
1:D:163:TRP:O	1:D:167:GLY:N	2.44	0.42
1:B:144:LEU:HD22	1:B:168:TRP:CZ2	2.54	0.42
1:B:210:GLU:HB3	1:B:211:TRP:CD2	2.55	0.42
1:D:221:GLN:NE2	1:D:225:ASP:OD1	2.51	0.42
1:D:153:GLU:HB3	1:D:277:ASN:ND2	2.35	0.42
1:D:568:PHE:O	1:D:572:ARG:HG2	2.20	0.42
1:A:134:ASN:HB2	1:A:163:TRP:CZ2	2.55	0.41
1:A:417:HIS:HB2	1:A:642:ASP:OD2	2.20	0.41
1:A:279:TYR:CE2	1:A:441:LYS:HB2	2.55	0.41
2:F:404:GLY:HA2	2:F:508:TYR:CD1	2.55	0.41
1:B:119:ILE:HG21	1:B:119:ILE:HD13	1.84	0.41
1:D:278:LEU:O	1:D:282:MET:HG2	2.20	0.41
1:A:153:GLU:HB3	1:A:277:ASN:ND2	2.36	0.41
2:E:354:ASN:O	2:E:398:ASP:HA	2.21	0.41
1:D:394:ASN:O	1:D:561:GLY:HA2	2.20	0.41
1:D:94:LYS:HE2	1:D:211:TRP:CE2	2.55	0.41
1:D:415:PRO:HG2	1:D:430:GLU:OE2	2.21	0.41
1:B:176:LEU:HD13	1:B:501:ALA:HB1	2.01	0.41
1:B:179:LEU:HD23	1:B:179:LEU:HA	1.72	0.41
1:B:244:VAL:HG23	1:B:282:MET:SD	2.61	0.41
1:D:392:LEU:HD13	1:D:563:SER:HA	2.01	0.41
1:D:24:LEU:HD21	2:F:476:GLY:HA2	2.03	0.41
1:A:117:ASN:O	1:A:121:ASN:HB2	2.21	0.41
1:A:641:CYS:SG	1:A:642:ASP:N	2.94	0.41
2:E:387:LEU:HA	2:E:387:LEU:HD23	1.81	0.41
1:B:453:THR:HG23	1:B:512:PHE:CD2	2.55	0.41
1:D:520:ILE:HG21	1:D:579:MET:HE3	2.02	0.41
1:A:341:LYS:HD3	1:A:341:LYS:HA	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:VAL:HA	1:B:229:THR:HG22	2.03	0.41
1:D:85:LEU:HD12	1:D:85:LEU:HA	1.86	0.41
2:F:338:PHE:HE2	2:F:363:ALA:HB1	1.85	0.41
2:E:502:GLY:O	2:E:506:GLN:HG3	2.21	0.40
1:B:284:PRO:HD2	1:B:437:ASN:OD1	2.22	0.40
1:B:335:GLU:HA	1:B:336:PRO:HD3	1.94	0.40
1:D:100:LEU:HD23	1:D:100:LEU:HA	1.84	0.40
1:A:177:ARG:HD3	1:A:497:TYR:O	2.22	0.40
1:A:332:MET:HE2	1:A:342:VAL:HG11	2.03	0.40
1:B:134:ASN:HB3	1:B:137:ASN:O	2.22	0.40
1:B:478:TRP:CD2	1:B:489:GLU:HB3	2.56	0.40
2:C:398:ASP:O	2:C:511:VAL:HA	2.21	0.40
2:C:394:ASN:HB3	2:C:396:TYR:HE1	1.87	0.40
1:D:557:MET:HE3	1:D:557:MET:HB2	1.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	594/597 (100%)	574 (97%)	19 (3%)	1 (0%)	47	81
1	B	594/597 (100%)	574 (97%)	19 (3%)	1 (0%)	47	81
1	D	594/597 (100%)	574 (97%)	20 (3%)	0	100	100
2	C	183/197 (93%)	176 (96%)	7 (4%)	0	100	100
2	E	181/197 (92%)	167 (92%)	14 (8%)	0	100	100
2	F	195/197 (99%)	183 (94%)	12 (6%)	0	100	100
All	All	2341/2382 (98%)	2248 (96%)	91 (4%)	2 (0%)	51	85

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	146	PRO
1	A	146	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	524/525 (100%)	476 (91%)	48 (9%)	9	32
1	B	524/525 (100%)	478 (91%)	46 (9%)	10	34
1	D	524/525 (100%)	483 (92%)	41 (8%)	12	40
2	C	161/170 (95%)	152 (94%)	9 (6%)	21	54
2	E	159/170 (94%)	136 (86%)	23 (14%)	3	14
2	F	170/170 (100%)	158 (93%)	12 (7%)	14	44
All	All	2062/2085 (99%)	1883 (91%)	179 (9%)	10	35

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	SER
1	A	21	THR
1	A	27	THR
1	A	44	SER
1	A	45	LEU
1	A	68	LYS
1	A	85	LEU
1	A	89	GLN
1	A	100	LEU
1	A	121	ASN
1	A	131	LYS
1	A	145	GLU
1	A	163	TRP
1	A	170	SER
1	A	183	TYR
1	A	210	GLU
1	A	231	THR

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Mol	Chain	Res	Type
1	A	238	GLU
1	A	244	VAL
1	A	283	VAL
1	A	287	GLN
1	A	317	SER
1	A	332	MET
1	A	343	VAL
1	A	381	TYR
1	A	385	TYR
1	A	394	ASN
1	A	401	HIS
1	A	407	ILE
1	A	409	SER
1	A	424	LEU
1	A	430	GLU
1	A	447	VAL
1	A	455	MET
1	A	460	ARG
1	A	476	LYS
1	A	495	GLU
1	A	496	THR
1	A	503	LEU
1	A	514	ARG
1	A	628	LEU
1	A	656	MET
1	A	669	LEU
1	A	676	LYS
1	A	677	THR
1	A	681	ARG
1	A	695	LYS
1	A	696	GLU
2	E	335	LEU
2	E	340	GLU
2	E	346	ARG
2	E	349	SER
2	E	354	ASN
2	E	359	SER
2	E	365	TYR
2	E	377	PHE
2	E	382	VAL
2	E	386	LYS
2	E	390	LEU

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Mol	Chain	Res	Type
2	E	391	CYS
2	E	393	THR
2	E	402	ILE
2	E	408	ARG
2	E	436	TRP
2	E	445	VAL
2	E	458	LYS
2	E	477	SER
2	E	478	THR
2	E	480	CYS
2	E	517	LEU
2	E	525	CYS
1	B	21	THR
1	B	26	LYS
1	B	56	ASP
1	B	60	GLN
1	B	74	GLU
1	B	76	GLU
1	B	82	THR
1	B	94	LYS
1	B	106	SER
1	B	107	VAL
1	B	111	ASP
1	B	121	ASN
1	B	125	THR
1	B	131	LYS
1	B	163	TRP
1	B	170	SER
1	B	171	GLU
1	B	198	ASP
1	B	211	TRP
1	B	224	GLU
1	B	227	GLU
1	B	231	THR
1	B	234	LYS
1	B	276	THR
1	B	282	MET
1	B	317	SER
1	B	334	THR
1	B	339	ASN
1	B	343	VAL
1	B	360	MET

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Mol	Chain	Res	Type
1	B	364	VAL
1	B	381	TYR
1	B	401	HIS
1	B	407	ILE
1	B	409	SER
1	B	424	LEU
1	B	432	SER
1	B	447	VAL
1	B	455	MET
1	B	518	ARG
1	B	522	GLN
1	B	529	LEU
1	B	570	LEU
1	B	578	THR
1	B	584	LEU
1	B	608	THR
2	C	333	THR
2	C	377	PHE
2	C	393	THR
2	C	430	THR
2	C	478	THR
2	C	493	GLN
2	C	494	SER
2	C	500	THR
2	C	514	SER
1	D	19	SER
1	D	21	THR
1	D	45	LEU
1	D	55	THR
1	D	59	ILE
1	D	77	SER
1	D	85	LEU
1	D	92	ILE
1	D	102	GLN
1	D	105	SER
1	D	106	SER
1	D	116	LEU
1	D	143	LEU
1	D	163	TRP
1	D	183	TYR
1	D	245	ARG
1	D	266	LEU

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Mol	Chain	Res	Type
1	D	276	THR
1	D	283	VAL
1	D	305	ARG
1	D	334	THR
1	D	341	LYS
1	D	342	VAL
1	D	343	VAL
1	D	354	HIS
1	D	364	VAL
1	D	381	TYR
1	D	385	TYR
1	D	394	ASN
1	D	401	HIS
1	D	424	LEU
1	D	455	MET
1	D	456	LEU
1	D	514	ARG
1	D	532	ILE
1	D	556	GLU
1	D	557	MET
1	D	570	LEU
1	D	573	VAL
1	D	578	THR
1	D	579	MET
2	F	334	ASN
2	F	341	VAL
2	F	376	THR
2	F	383	SER
2	F	403	ARG
2	F	415	THR
2	F	424	LYS
2	F	436	TRP
2	F	478	THR
2	F	480	CYS
2	F	495	TYR
2	F	503	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z|>2$	Counts	RMSZ	#$|Z|>2$
3	NAG	G	1	3,1	14,14,15	1.03	1 (7%)	17,19,21	0.86	1 (5%)
3	NAG	G	2	3	14,14,15	0.94	1 (7%)	17,19,21	1.22	2 (11%)
4	NAG	H	1	4,1	14,14,15	1.39	2 (14%)	17,19,21	0.84	1 (5%)
4	FUC	H	2	4	10,10,11	2.50	5 (50%)	14,14,16	1.62	4 (28%)
3	NAG	I	1	3,1	14,14,15	0.38	0	17,19,21	0.63	0
3	NAG	I	2	3	14,14,15	0.30	0	17,19,21	0.94	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	3/6/23/26	0/1/1/1
4	NAG	H	1	4,1	-	0/6/23/26	0/1/1/1
4	FUC	H	2	4	-	-	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	3/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	2	FUC	C4-C5	3.86	1.61	1.52
4	H	2	FUC	C4-C3	3.70	1.61	1.52
3	G	1	NAG	O5-C1	3.57	1.49	1.43
4	H	1	NAG	C1-C2	3.52	1.57	1.52
4	H	1	NAG	O5-C1	3.51	1.49	1.43
4	H	2	FUC	C2-C3	3.22	1.57	1.52
4	H	2	FUC	C1-C2	3.16	1.59	1.52
4	H	2	FUC	O5-C5	2.77	1.49	1.43
3	G	2	NAG	C1-C2	2.66	1.56	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	2	NAG	C2-N2-C7	3.41	127.76	122.90
4	H	2	FUC	O5-C5-C4	3.07	115.03	109.52
3	G	2	NAG	C1-C2-N2	2.77	115.22	110.49
3	G	1	NAG	C1-O5-C5	2.58	115.69	112.19
4	H	2	FUC	C1-C2-C3	2.55	112.80	109.67
4	H	1	NAG	C1-O5-C5	2.47	115.54	112.19
4	H	2	FUC	C1-O5-C5	2.31	118.01	112.78
3	I	2	NAG	C1-O5-C5	2.16	115.12	112.19
4	H	2	FUC	O2-C2-C1	2.09	113.43	109.15

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C1-C2-N2-C7
3	I	2	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 G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings
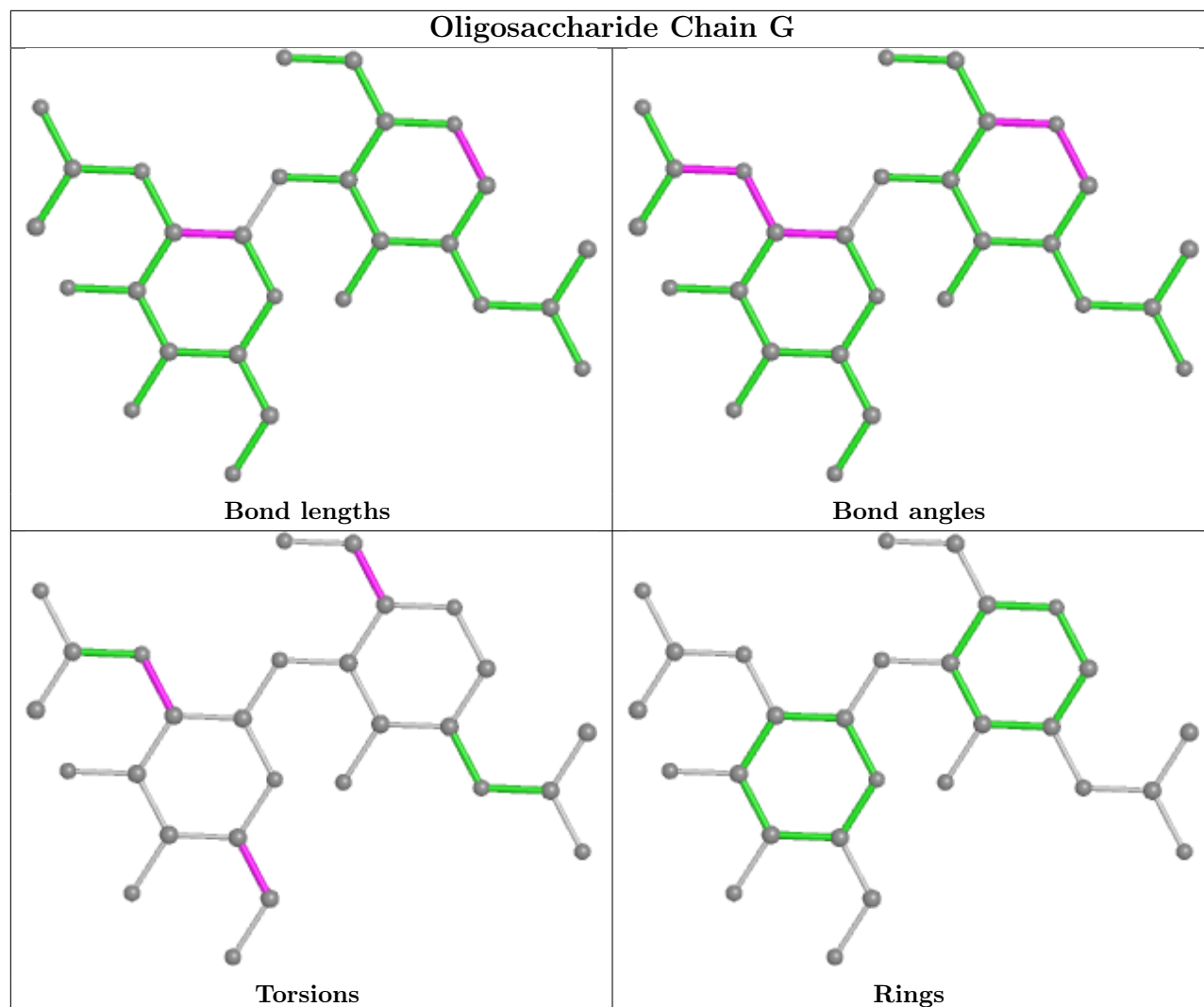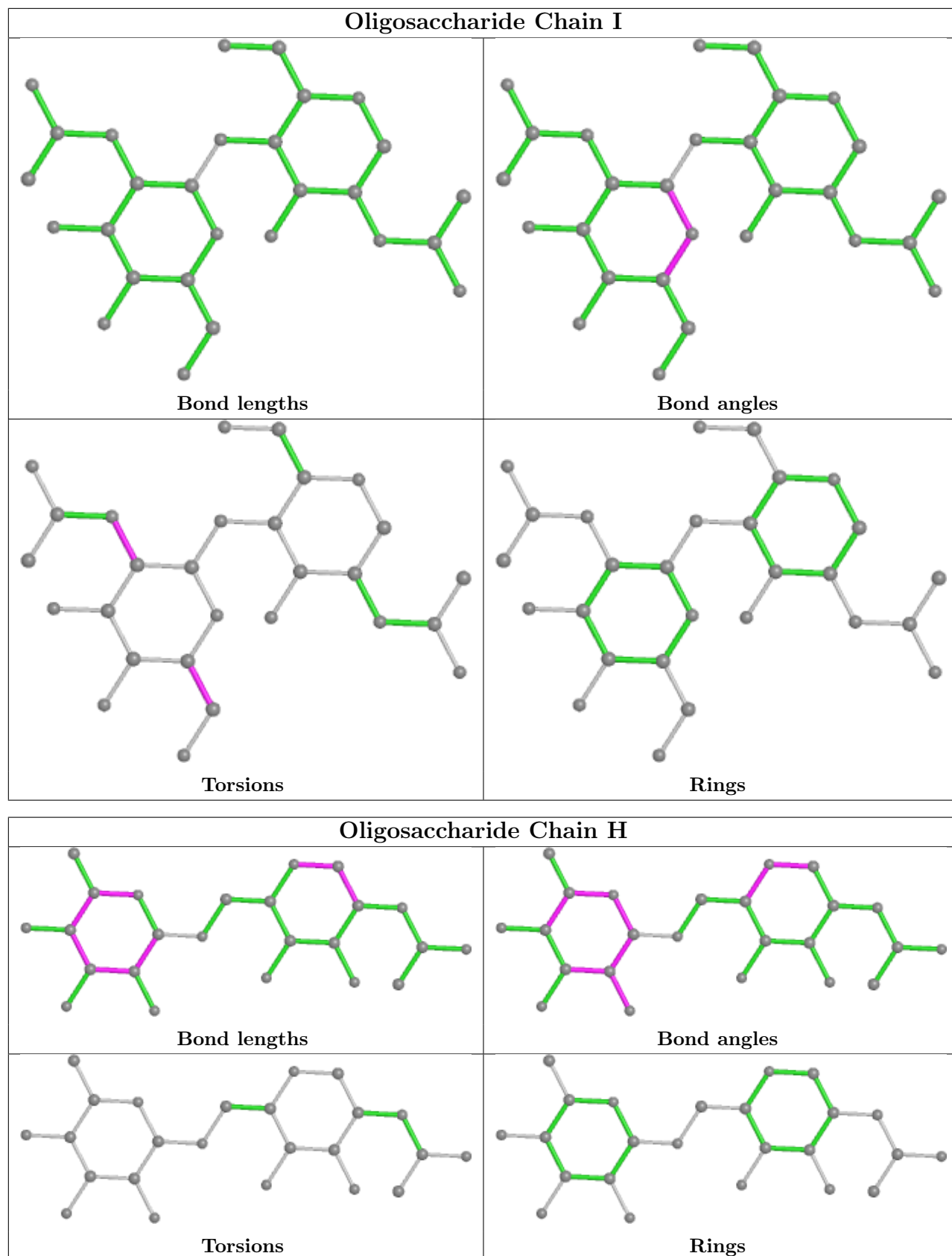
5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
5	NAG	B	903	1	14,14,15	1.91	2 (14%)	17,19,21	1.26	2 (11%)
5	NAG	E	601	2	14,14,15	1.84	1 (7%)	17,19,21	1.56	4 (23%)
5	NAG	B	905	1	14,14,15	1.96	2 (14%)	17,19,21	0.90	1 (5%)
5	NAG	D	903	1	14,14,15	1.16	2 (14%)	17,19,21	0.58	0
5	NAG	B	904	1	14,14,15	0.55	0	17,19,21	0.95	1 (5%)
5	NAG	A	903	1	14,14,15	0.64	0	17,19,21	1.07	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
5	NAG	B	903	1	-	2/6/23/26	0/1/1/1
5	NAG	E	601	2	-	2/6/23/26	0/1/1/1
5	NAG	B	905	1	-	2/6/23/26	0/1/1/1
5	NAG	D	903	1	-	2/6/23/26	0/1/1/1
5	NAG	B	904	1	-	2/6/23/26	0/1/1/1
5	NAG	A	903	1	-	3/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	601	NAG	O5-C1	6.65	1.54	1.43
5	B	905	NAG	O5-C1	6.29	1.53	1.43
5	B	903	NAG	O5-C1	5.88	1.53	1.43
5	B	903	NAG	C1-C2	3.69	1.57	1.52
5	B	905	NAG	C1-C2	3.46	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	903	NAG	C1-C2	3.24	1.57	1.52
5	D	903	NAG	O5-C1	2.65	1.47	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	601	NAG	C1-O5-C5	3.94	117.53	112.19
5	B	903	NAG	C1-O5-C5	3.69	117.19	112.19
5	B	904	NAG	C1-O5-C5	3.35	116.73	112.19
5	E	601	NAG	C2-N2-C7	2.85	126.96	122.90
5	B	905	NAG	C1-O5-C5	2.69	115.84	112.19
5	E	601	NAG	C1-C2-N2	2.44	114.66	110.49
5	A	903	NAG	C1-O5-C5	2.41	115.46	112.19
5	E	601	NAG	C4-C3-C2	-2.07	107.99	111.02
5	B	903	NAG	O6-C6-C5	2.03	118.27	111.29

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	903	NAG	O5-C5-C6-O6
5	A	903	NAG	C4-C5-C6-O6
5	D	903	NAG	O5-C5-C6-O6
5	B	904	NAG	O5-C5-C6-O6
5	D	903	NAG	C4-C5-C6-O6
5	B	904	NAG	C4-C5-C6-O6
5	B	905	NAG	C4-C5-C6-O6
5	B	903	NAG	C4-C5-C6-O6
5	E	601	NAG	O5-C5-C6-O6
5	B	905	NAG	O5-C5-C6-O6
5	B	903	NAG	O5-C5-C6-O6
5	E	601	NAG	C3-C2-N2-C7
5	A	903	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	904	NAG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6　Fit of model and data ⓘ

6.1　Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	596/597 (99%)	-0.34	3 (0%)	91	75	44, 60, 87, 114	0
1	B	596/597 (99%)	-0.35	1 (0%)	95	87	42, 62, 92, 133	0
1	D	596/597 (99%)	-0.31	6 (1%)	82	58	48, 70, 94, 132	0
2	C	187/197 (94%)	-0.34	1 (0%)	91	75	43, 53, 100, 140	0
2	E	185/197 (93%)	-0.27	5 (2%)	54	26	44, 55, 98, 145	0
2	F	197/197 (100%)	-0.41	0	100	100	46, 58, 87, 111	0
All	All	2357/2382 (98%)	-0.34	16 (0%)	87	68	42, 63, 94, 145	0

All (16) RSRZ outliers are listed below:

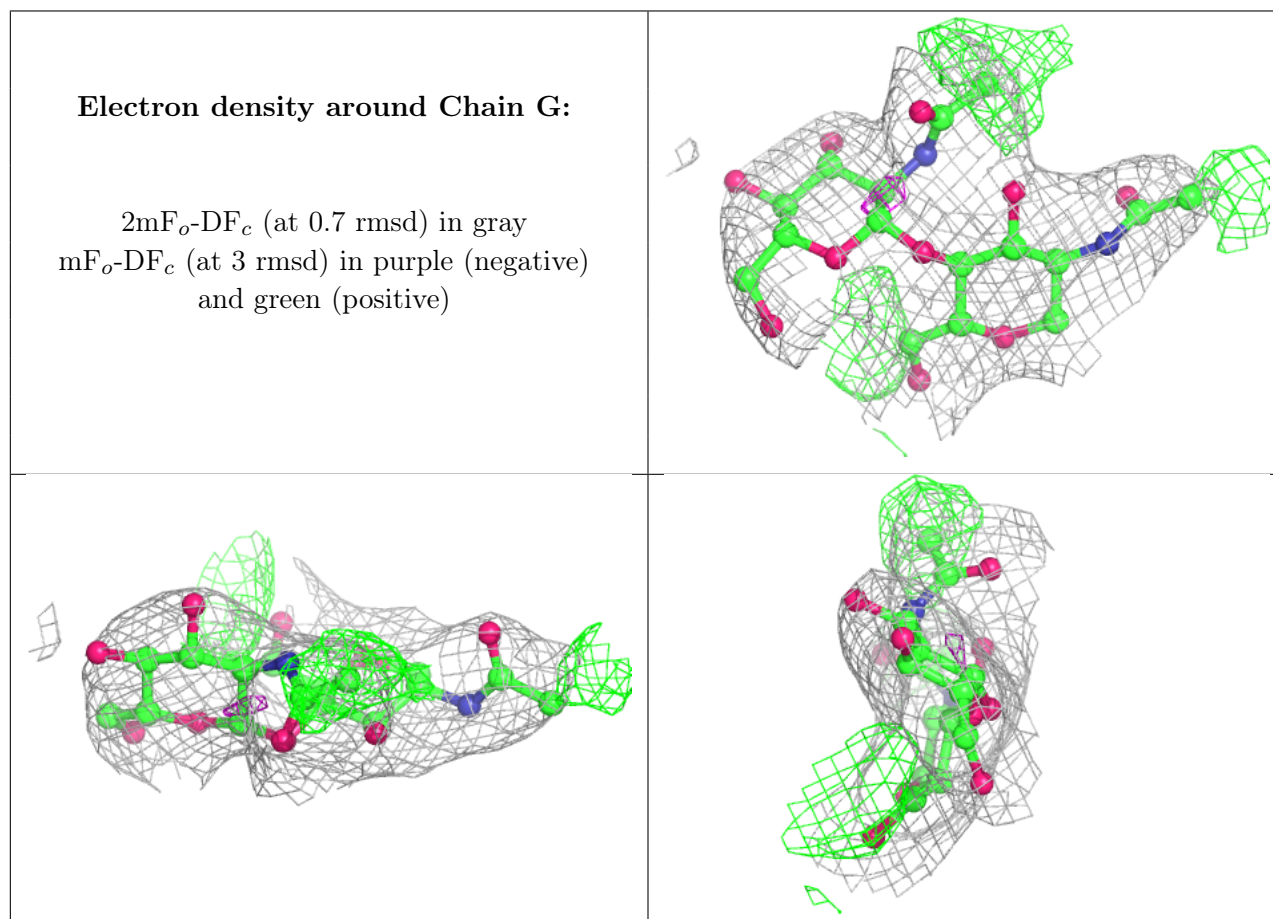| Mol	Chain	Res	Type	RSRZ
1	D	211	TRP	3.2
1	A	339	ASN	3.0
1	D	339	ASN	3.0
1	B	338	ASP	2.9
1	D	341	LYS	2.7
2	C	333	THR	2.7
2	E	519	HIS	2.4
2	E	362	VAL	2.4
1	A	337	GLY	2.2
1	A	341	LYS	2.2
1	D	427	ASP	2.2
2	E	518	LEU	2.1
1	D	140	GLU	2.1
2	E	391	CYS	2.1
1	D	139	GLN	2.0
2	E	338	PHE	2.0

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, 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.
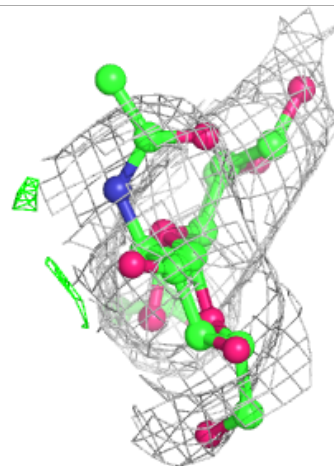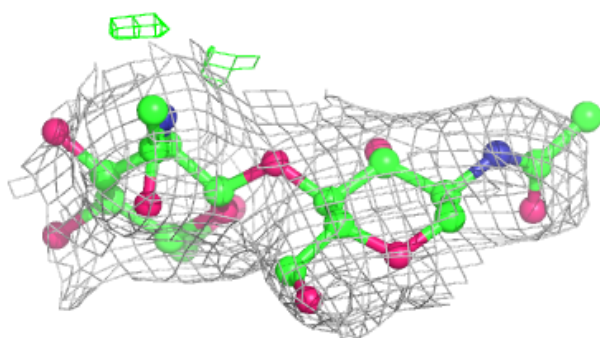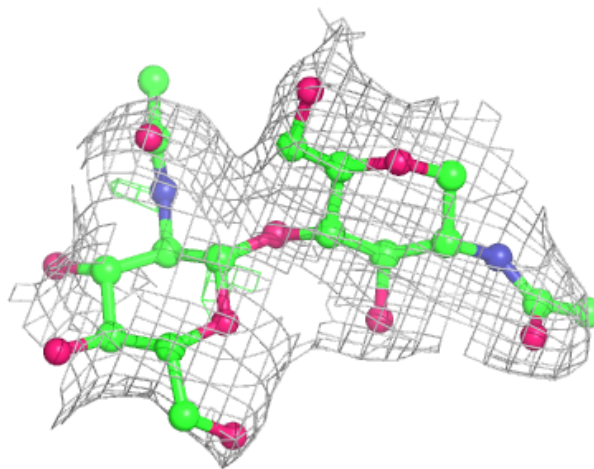
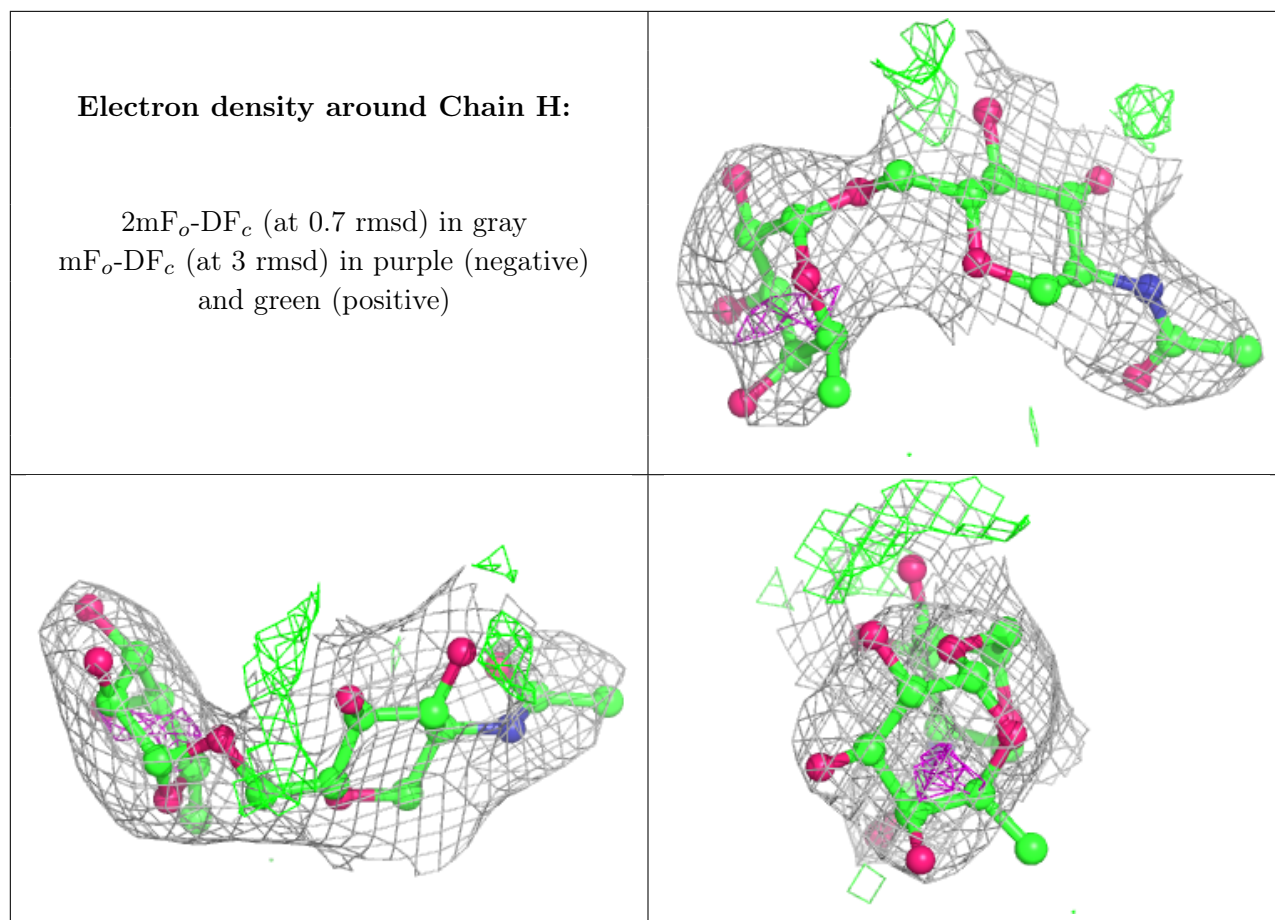| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\mathring{A}^2$)	Q<0.9
3	NAG	I	2	14/15	0.80	0.37	117,126,134,138	0
3	NAG	G	2	14/15	0.82	0.24	87,105,109,110	0
3	NAG	G	1	14/15	0.86	0.16	67,87,98,107	0
4	NAG	H	1	14/15	0.86	0.28	71,85,97,105	0
4	FUC	H	2	10/11	0.93	0.46	86,99,102,102	0
3	NAG	I	1	14/15	0.95	0.35	81,87,104,119	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 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 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 ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
5	NAG	E	601	14/15	0.55	0.31	104,122,127,130	0
5	NAG	B	905	14/15	0.75	0.30	75,89,93,97	0
5	NAG	B	903	14/15	0.78	0.19	56,74,83,83	0
5	NAG	D	903	14/15	0.82	0.30	100,115,118,122	0
5	NAG	B	904	14/15	0.89	0.31	74,78,84,86	0
5	NAG	A	903	14/15	0.92	0.35	72,81,87,88	0

6.5 Other polymers ⓘ

There are no such residues in this entry.