



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:07 PM UTC

PDB ID : 4JUH / pdb_00004juh
Title : Crystal structure of 1918 pandemic influenza virus hemagglutinin mutant D225G complexed with avian receptor analogue LSTa
Authors : Zhang, W.; Shi, Y.; Qi, J.; Gao, F.; Li, Q.; Fan, Z.; Yan, J.; Gao, G.F.
Deposited on : 2013-03-24
Resolution : 2.81 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:

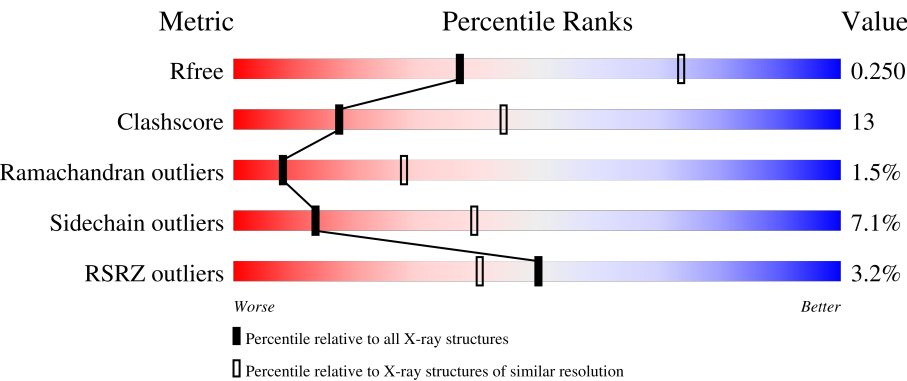
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.81 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	324	0% 78%19%.
1	C	324	2% 78%19%.
1	E	324	2% 81%16%.
2	B	170	4% 69%24%6%.
2	D	170	8% 66%24%. . .

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Mol	Chain	Length	Quality of chain
2	F	170	7% 70% 21%
3	G	2	50% 50%
3	I	2	50% 50%
3	J	2	50% 50%
4	H	3	33% 33% 33%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11875 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2512	1584	434	483	11			
1	C	324	Total	C	N	O	S	0	0	0
			2512	1584	434	483	11			
1	E	324	Total	C	N	O	S	0	0	0
			2512	1584	434	483	11			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	GLY	ASP	engineered mutation	UNP Q9WFX3
A	326	ALA	-	expression tag	UNP Q9WFX3
A	327	ARG	-	expression tag	UNP Q9WFX3
C	225	GLY	ASP	engineered mutation	UNP Q9WFX3
C	326	ALA	-	expression tag	UNP Q9WFX3
C	327	ARG	-	expression tag	UNP Q9WFX3
E	225	GLY	ASP	engineered mutation	UNP Q9WFX3
E	326	ALA	-	expression tag	UNP Q9WFX3
E	327	ARG	-	expression tag	UNP Q9WFX3

- Molecule 2 is a protein called Hemagglutinin.

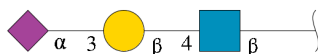
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	170	Total	C	N	O	S	0	0	0
			1368	855	236	271	6			
2	D	164	Total	C	N	O	S	0	0	0
			1317	825	225	261	6			
2	F	165	Total	C	N	O	S	0	0	0
			1326	830	226	264	6			

- Molecule 3 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
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	3	Total	C	N	O	0	0	0
			45	25	2	18			

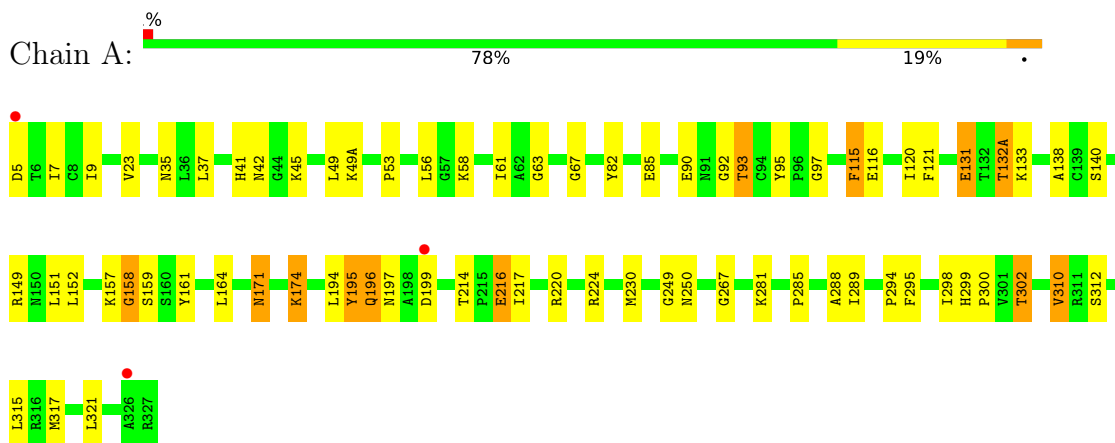
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	53	Total	O	0	0
			53	53		
5	B	23	Total	O	0	0
			23	23		
5	C	51	Total	O	0	0
			51	51		
5	D	9	Total	O	0	0
			9	9		
5	E	46	Total	O	0	0
			46	46		
5	F	17	Total	O	0	0
			17	17		

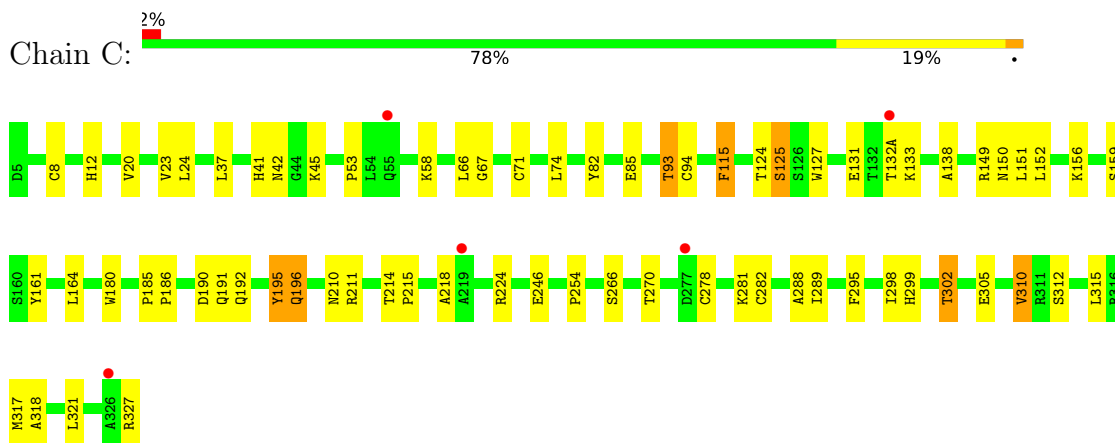
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

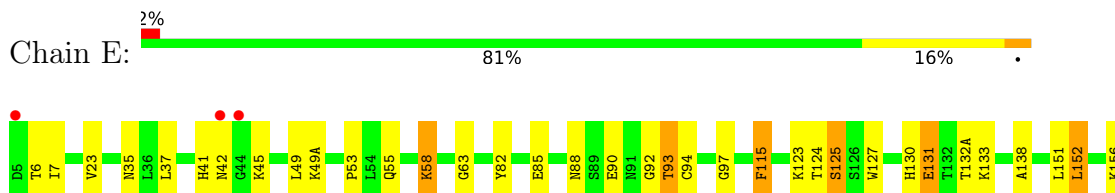
• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin

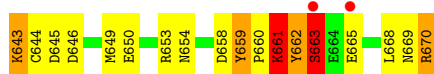


• Molecule 1: Hemagglutinin

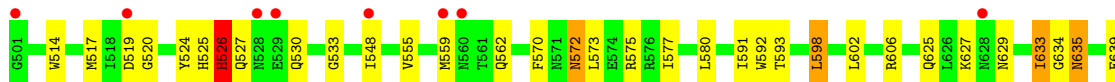




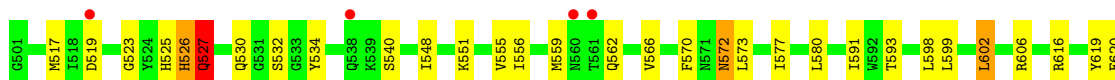
• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



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



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





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

Chain J:



- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.99Å 243.19Å 72.21Å 90.00° 119.62° 90.00°	Depositor
Resolution (Å)	38.40 – 2.81 38.40 – 2.81	Depositor EDS
% Data completeness (in resolution range)	94.4 (38.40-2.81) 99.4 (38.40-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.201 , 0.246 0.203 , 0.250	Depositor DCC
R_{free} test set	2671 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h-l,k,h 0.000 for l,k,-h-l 0.019 for h,-k,-h-l 0.021 for -h-l,-k,l 0.022 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11875	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, GAL, 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	0.37	0/2576	0.82	7/3508 (0.2%)
1	C	0.32	0/2576	0.81	6/3508 (0.2%)
1	E	0.31	0/2576	0.79	5/3508 (0.1%)
2	B	0.56	1/1395 (0.1%)	0.97	9/1878 (0.5%)
2	D	0.40	0/1344	0.79	5/1811 (0.3%)
2	F	0.37	0/1353	0.81	7/1823 (0.4%)
All	All	0.38	1/11820 (0.0%)	0.83	39/16036 (0.2%)

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
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	661	LYS	N-CA	-5.09	1.39	1.46

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	525	HIS	CB-CA-C	-18.62	83.43	110.62
1	C	195	TYR	CB-CA-C	12.89	131.77	110.24
1	A	196	GLN	CB-CA-C	-12.38	85.79	110.42
1	E	196	GLN	CB-CA-C	-12.02	86.50	110.42
2	F	657	TYR	N-CA-C	11.66	130.50	111.37
2	B	662	TYR	N-CA-C	11.62	127.92	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	663	SER	N-CA-C	11.31	126.61	113.15
1	A	195	TYR	CB-CA-C	9.54	124.13	109.34
1	C	196	GLN	CB-CA-C	-9.38	91.76	110.42
1	E	195	TYR	CB-CA-C	9.10	123.45	109.34
2	F	657	TYR	CB-CA-C	-8.27	97.11	110.84
1	E	196	GLN	N-CA-C	8.14	128.15	110.80
2	D	661	LYS	N-CA-C	7.65	122.02	109.24
1	A	196	GLN	N-CA-C	7.43	126.63	110.80
1	C	196	GLN	N-CA-C	7.11	125.94	110.80
2	B	627	LYS	CB-CA-C	-6.95	108.55	116.54
2	D	661	LYS	CB-CA-C	-6.56	96.35	109.35
2	D	658	ASP	N-CA-C	6.16	123.91	110.80
2	F	627	LYS	CB-CA-C	-6.14	109.51	116.63
2	D	627	LYS	CB-CA-C	-6.12	109.54	116.63
2	B	663	SER	CB-CA-C	-6.04	99.18	110.36
2	B	663	SER	CA-C-N	5.89	132.80	121.54
2	B	663	SER	C-N-CA	5.89	132.80	121.54
2	D	658	ASP	CB-CA-C	-5.54	99.39	110.42
2	F	659	TYR	CA-C-N	-5.51	112.95	119.84
2	F	659	TYR	C-N-CA	-5.51	112.95	119.84
1	A	196	GLN	CA-C-N	5.42	129.62	122.30
1	A	196	GLN	C-N-CA	5.42	129.62	122.30
1	C	299	HIS	CA-C-N	5.28	124.91	119.05
1	C	299	HIS	C-N-CA	5.28	124.91	119.05
2	F	657	TYR	CA-C-N	5.24	131.56	121.54
2	F	657	TYR	C-N-CA	5.24	131.56	121.54
1	C	195	TYR	N-CA-C	-5.21	105.75	112.68
2	B	659	TYR	CA-C-N	5.13	126.26	119.84
2	B	659	TYR	C-N-CA	5.13	126.26	119.84
1	A	132(A)	THR	CA-C-N	-5.12	117.39	126.45
1	A	132(A)	THR	C-N-CA	-5.12	117.39	126.45
1	E	127	TRP	CA-C-N	5.07	124.67	119.05
1	E	127	TRP	C-N-CA	5.07	124.67	119.05

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	663	SER	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	2512	0	2440	60	0
1	C	2512	0	2440	49	0
1	E	2512	0	2440	47	0
2	B	1368	0	1285	69	0
2	D	1317	0	1231	54	0
2	F	1326	0	1237	44	0
3	G	28	0	25	1	0
3	I	28	0	25	1	0
3	J	28	0	25	1	0
4	H	45	0	38	1	0
5	A	53	0	0	0	0
5	B	23	0	0	1	0
5	C	51	0	0	0	0
5	D	9	0	0	2	0
5	E	46	0	0	1	0
5	F	17	0	0	0	0
All	All	11875	0	11186	286	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 13.

All (286) 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:D:663:SER:HA	2:D:664:GLU:CB	1.56	1.31
1:A:131:GLU:OE1	1:A:133:LYS:HD2	1.28	1.29
2:F:526:HIS:HE1	2:F:532:SER:C	1.44	1.25
2:D:663:SER:HA	2:D:664:GLU:HB2	1.12	1.11
2:D:662:TYR:O	2:D:663:SER:HB3	1.45	1.10
2:D:658:ASP:O	2:D:658:ASP:OD2	1.67	1.09
1:E:6:THR:O	2:F:526:HIS:O	1.70	1.09
2:D:663:SER:CA	2:D:664:GLU:CB	2.30	1.08
2:F:526:HIS:CE1	2:F:532:SER:C	2.36	1.04
2:D:663:SER:CB	2:D:664:GLU:HB3	1.91	1.01
2:D:663:SER:CA	2:D:664:GLU:HB3	1.90	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:663:SER:HA	2:D:664:GLU:HB3	1.46	0.97
2:B:526:HIS:CD2	2:B:649:MET:HG3	2.00	0.96
2:B:659:TYR:HB3	2:B:660:PRO:HD3	1.45	0.95
2:B:669:ASN:C	2:B:670:ARG:HG3	1.91	0.95
2:D:663:SER:HB2	2:D:664:GLU:HB3	1.48	0.94
1:A:131:GLU:OE1	1:A:133:LYS:CD	2.14	0.94
1:A:132(A):THR:O	1:A:133:LYS:HB2	1.65	0.94
2:F:662:TYR:CE1	2:F:664:GLU:OE2	2.23	0.92
2:D:662:TYR:O	2:D:663:SER:CB	2.22	0.88
2:D:525:HIS:O	2:D:533:GLY:O	1.92	0.85
1:E:195:TYR:O	1:E:196:GLN:HB2	1.74	0.85
2:D:517:MET:HB3	5:D:702:HOH:O	1.76	0.85
2:D:526:HIS:O	2:D:526:HIS:CD2	2.30	0.85
2:D:526:HIS:O	2:D:526:HIS:CG	2.30	0.84
2:D:650:GLU:O	2:D:654:ASN:HB2	1.79	0.81
2:D:658:ASP:OD2	2:D:658:ASP:C	2.23	0.80
2:F:662:TYR:HE1	2:F:664:GLU:OE2	1.65	0.80
2:F:526:HIS:ND1	2:F:527:GLN:N	2.29	0.80
1:A:195:TYR:O	1:A:196:GLN:CB	2.27	0.79
1:A:196:GLN:HG2	1:A:196:GLN:O	1.82	0.79
2:B:662:TYR:O	2:B:665:GLU:CG	2.32	0.78
2:B:526:HIS:CE1	2:B:653:ARG:NH2	2.53	0.77
2:B:659:TYR:HB3	2:B:660:PRO:CD	2.14	0.77
2:B:530:GLN:HE22	2:B:646:ASP:H	1.33	0.76
2:B:662:TYR:O	2:B:665:GLU:HG3	1.86	0.74
1:C:196:GLN:HG3	1:C:196:GLN:O	1.87	0.74
1:C:310:VAL:HG13	1:C:312:SER:H	1.50	0.74
2:B:663:SER:HA	2:B:665:GLU:HG3	1.69	0.73
2:F:662:TYR:CD1	2:F:664:GLU:OE2	2.42	0.73
1:C:156:LYS:HB3	1:C:195:TYR:O	1.88	0.72
2:B:660:PRO:O	2:B:661:LYS:C	2.30	0.72
2:B:629:ASN:ND2	2:B:665:GLU:HG2	2.05	0.71
1:C:317:MET:HE1	2:D:555:VAL:HG21	1.71	0.71
2:B:661:LYS:HB3	2:B:662:TYR:CD2	2.26	0.71
2:F:526:HIS:CE1	2:F:532:SER:O	2.44	0.71
2:B:526:HIS:ND1	2:B:653:ARG:NH2	2.39	0.70
1:A:41:HIS:HB3	1:A:298:ILE:HD13	1.73	0.69
2:B:659:TYR:N	2:B:660:PRO:CD	2.54	0.69
2:F:526:HIS:HE1	2:F:532:SER:O	1.75	0.68
1:C:295:PHE:CZ	2:D:559:MET:HE2	2.29	0.68
2:D:514:TRP:HB2	5:D:702:HOH:O	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:526:HIS:HE1	2:F:532:SER:CA	2.06	0.67
1:E:41:HIS:HB3	1:E:298:ILE:HD13	1.77	0.67
1:E:310:VAL:HG13	1:E:312:SER:H	1.59	0.67
2:B:629:ASN:HB3	2:B:642:HIS:HD2	1.59	0.66
1:A:310:VAL:HG13	1:A:312:SER:H	1.61	0.66
2:B:633:ILE:HG22	2:B:634:GLY:N	2.10	0.65
2:B:528:ASN:HD22	2:B:529:GLU:N	1.95	0.65
1:A:195:TYR:O	1:A:196:GLN:HB3	1.97	0.64
2:B:526:HIS:CE1	2:B:653:ARG:HH22	2.16	0.64
2:B:660:PRO:O	2:B:662:TYR:N	2.32	0.63
2:B:628:ASN:HB2	2:B:659:TYR:OH	1.99	0.63
2:B:650:GLU:O	2:B:654:ASN:HB2	1.97	0.63
2:B:665:GLU:O	2:B:669:ASN:HB2	2.00	0.62
1:A:195:TYR:O	1:A:196:GLN:HB2	1.98	0.62
1:A:285:PRO:HG2	1:A:299:HIS:CE1	2.34	0.62
2:B:528:ASN:HD22	2:B:529:GLU:H	1.46	0.62
2:B:660:PRO:C	2:B:662:TYR:N	2.55	0.61
2:B:528:ASN:ND2	2:B:530:GLN:HE21	1.98	0.61
2:B:658:ASP:OD2	2:B:660:PRO:HD2	2.00	0.61
1:A:171:ASN:H	1:A:171:ASN:HD22	1.49	0.60
1:C:93:THR:HG22	1:C:93:THR:O	2.00	0.60
1:E:132(A):THR:HG22	1:E:133:LYS:H	1.66	0.60
2:D:659:TYR:CE2	2:D:661:LYS:HD2	2.36	0.60
2:F:525:HIS:HD2	2:F:534:TYR:CE2	2.20	0.60
1:A:131:GLU:CD	1:A:133:LYS:HD2	2.22	0.59
2:B:629:ASN:N	2:B:629:ASN:HD22	1.98	0.59
1:E:295:PHE:CE2	2:F:559:MET:HE2	2.37	0.59
1:E:131:GLU:OE1	1:E:133:LYS:HD2	2.02	0.59
1:C:302:THR:HB	2:D:562:GLN:HE21	1.66	0.59
2:B:530:GLN:NE2	2:B:646:ASP:H	2.00	0.59
1:C:295:PHE:HZ	2:D:559:MET:HE2	1.68	0.58
2:D:526:HIS:CD2	2:D:526:HIS:C	2.80	0.58
1:C:41:HIS:HB3	1:C:298:ILE:HD13	1.85	0.58
2:B:659:TYR:CB	2:B:660:PRO:HD3	2.15	0.58
1:A:93:THR:HG22	1:A:93:THR:O	2.03	0.57
2:B:528:ASN:ND2	2:B:529:GLU:H	2.02	0.57
1:A:37:LEU:HB2	1:A:315:LEU:HB2	1.85	0.57
2:B:628:ASN:ND2	2:B:659:TYR:OH	2.38	0.57
1:E:185:PRO:HG2	1:E:191:GLN:NE2	2.20	0.57
1:A:295:PHE:CZ	2:B:559:MET:HE2	2.39	0.57
2:B:660:PRO:C	2:B:662:TYR:H	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:LEU:HD11	4:H:3:SIA:H92	1.86	0.57
1:C:20:VAL:HG11	1:C:318:ALA:HB2	1.87	0.57
1:E:123:LYS:HG3	1:E:152:LEU:HD11	1.85	0.57
1:C:42:ASN:ND2	1:C:45:LYS:HB2	2.20	0.56
1:C:310:VAL:HG22	2:D:593:THR:HA	1.87	0.56
2:F:629:ASN:ND2	2:F:659:TYR:HE1	2.02	0.56
1:A:161:TYR:HB2	1:A:195:TYR:O	2.04	0.56
2:D:641:TYR:CE1	2:D:664:GLU:HG3	2.40	0.56
1:A:7:ILE:HA	2:B:526:HIS:HA	1.87	0.56
1:A:302:THR:HB	2:B:562:GLN:HE21	1.70	0.56
1:E:302:THR:HB	2:F:562:GLN:HE21	1.68	0.56
1:C:161:TYR:HB2	1:C:195:TYR:O	2.06	0.56
1:C:224:ARG:NH2	3:I:1:NAG:O3	2.40	0.55
2:B:642:HIS:O	2:B:643:LYS:HB3	2.07	0.55
1:C:37:LEU:HB2	1:C:315:LEU:HB2	1.88	0.55
1:C:138:ALA:O	1:C:224:ARG:NH1	2.40	0.55
1:E:97:GLY:HA3	1:E:230:MET:O	2.07	0.54
2:F:650:GLU:O	2:F:654:ASN:HB2	2.07	0.54
1:C:186:PRO:HA	1:C:218:ALA:O	2.07	0.54
2:D:570:PHE:CE1	2:D:577:ILE:HG22	2.43	0.54
1:C:132(A):THR:HG22	1:C:133:LYS:H	1.72	0.54
1:E:161:TYR:HB2	1:E:195:TYR:O	2.08	0.54
1:A:164:LEU:C	1:A:164:LEU:HD12	2.33	0.54
2:F:530:GLN:HE21	2:F:645:ASP:HB2	1.73	0.54
1:A:216:GLU:HG2	1:C:211:ARG:HA	1.89	0.53
1:C:42:ASN:HB3	1:C:288:ALA:H	1.73	0.53
1:C:124:THR:O	1:C:125:SER:HB2	2.08	0.53
1:E:42:ASN:HB3	1:E:288:ALA:H	1.72	0.53
1:E:138:ALA:O	1:E:224:ARG:NH1	2.41	0.53
1:E:196:GLN:O	1:E:196:GLN:OE1	2.26	0.53
2:F:526:HIS:CE1	2:F:532:SER:CA	2.86	0.53
2:F:530:GLN:NE2	2:F:645:ASP:HB2	2.23	0.53
2:D:591:ILE:HD13	2:F:591:ILE:HG21	1.90	0.52
1:A:171:ASN:H	1:A:171:ASN:ND2	2.06	0.52
1:E:224:ARG:NH2	3:J:1:NAG:O3	2.42	0.52
1:A:295:PHE:CE2	2:B:559:MET:HE2	2.45	0.52
1:C:124:THR:O	1:C:125:SER:CB	2.57	0.52
2:F:526:HIS:CE1	2:F:532:SER:HA	2.45	0.52
1:E:294:PRO:HG3	2:F:556:ILE:HG12	1.91	0.52
2:F:517:MET:SD	2:F:523:GLY:HA3	2.50	0.52
2:D:656:THR:C	2:D:657:TYR:O	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ALA:O	1:A:224:ARG:NH1	2.43	0.52
1:A:321:LEU:HD23	1:A:321:LEU:H	1.75	0.52
2:D:633:ILE:HD11	2:D:639:GLU:HB2	1.91	0.52
1:E:295:PHE:CZ	2:F:559:MET:HE2	2.44	0.52
2:D:661:LYS:C	2:D:662:TYR:CD1	2.88	0.52
1:E:124:THR:O	1:E:125:SER:HB2	2.10	0.51
1:A:56:LEU:HD12	1:A:85:GLU:HG2	1.93	0.51
2:B:606:ARG:HH12	2:F:606:ARG:HH11	1.58	0.51
2:D:559:MET:HE1	2:D:592:TRP:CZ3	2.46	0.51
2:B:659:TYR:N	2:B:660:PRO:HD3	2.27	0.50
1:E:132(A):THR:HG23	5:E:914:HOH:O	2.11	0.50
1:A:289:ILE:HD11	1:A:298:ILE:HD12	1.93	0.50
2:D:530:GLN:HE21	2:D:645:ASP:HB2	1.75	0.50
1:E:53:PRO:HB3	1:E:82:TYR:CE2	2.47	0.50
2:B:526:HIS:HD2	2:B:649:MET:HG3	1.71	0.50
1:C:85:GLU:O	1:C:270:THR:HA	2.10	0.50
1:E:310:VAL:HG22	2:F:593:THR:HA	1.94	0.50
2:B:606:ARG:HH11	2:D:606:ARG:NH1	2.10	0.50
1:C:164:LEU:O	1:C:246:GLU:HA	2.12	0.50
2:B:619:TYR:CE1	2:B:636:GLY:HA2	2.47	0.50
1:C:196:GLN:O	1:C:196:GLN:CG	2.56	0.50
2:D:629:ASN:N	2:D:629:ASN:HD22	2.10	0.50
2:D:656:THR:O	2:D:657:TYR:O	2.29	0.50
2:B:606:ARG:NH1	2:F:606:ARG:HH11	2.10	0.49
2:B:570:PHE:CE1	2:B:577:ILE:HG22	2.48	0.49
2:F:663:SER:O	2:F:663:SER:OG	2.30	0.49
1:E:42:ASN:ND2	1:E:45:LYS:HB2	2.27	0.49
1:A:7:ILE:HG13	2:B:526:HIS:HB3	1.94	0.49
1:E:223:VAL:HG12	1:E:224:ARG:HG3	1.93	0.49
2:B:661:LYS:HB3	2:B:662:TYR:CE2	2.47	0.49
1:C:282:CYS:HB2	1:C:305:GLU:O	2.13	0.48
1:A:56:LEU:HD11	1:A:61:ILE:HD13	1.95	0.48
2:D:663:SER:CA	2:D:664:GLU:HB2	2.06	0.48
1:E:93:THR:HG22	1:E:93:THR:O	2.12	0.48
2:F:616:ARG:O	2:F:620:GLU:HG3	2.12	0.48
1:A:310:VAL:HG22	2:B:593:THR:HA	1.95	0.48
1:E:94:CYS:O	1:E:224:ARG:HD3	2.14	0.48
1:C:185:PRO:HG2	1:C:191:GLN:NE2	2.28	0.47
1:E:156:LYS:HD2	1:E:196:GLN:HG2	1.96	0.47
1:A:42:ASN:HB3	1:A:288:ALA:H	1.79	0.47
1:A:97:GLY:HA3	1:A:230:MET:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:PHE:CE2	2:D:559:MET:HE2	2.50	0.47
2:F:662:TYR:O	2:F:663:SER:O	2.33	0.47
2:B:629:ASN:ND2	2:B:629:ASN:N	2.63	0.47
2:B:629:ASN:OD1	2:B:662:TYR:HB2	2.15	0.47
1:C:185:PRO:HG2	1:C:191:GLN:HE21	1.78	0.47
2:F:570:PHE:CE1	2:F:577:ILE:HG22	2.49	0.47
1:A:317:MET:HE1	2:B:555:VAL:HG21	1.97	0.46
1:C:12:HIS:HB2	2:D:520:GLY:O	2.15	0.46
2:F:619:TYR:CE1	2:F:636:GLY:HA2	2.51	0.46
2:F:572:ASN:C	2:F:572:ASN:HD22	2.21	0.46
2:D:530:GLN:NE2	2:D:646:ASP:H	2.14	0.46
2:F:526:HIS:CG	2:F:527:GLN:N	2.84	0.46
1:A:116:GLU:OE1	1:A:174:LYS:NZ	2.48	0.46
1:E:195:TYR:O	1:E:196:GLN:CB	2.55	0.46
1:A:249:GLY:C	1:A:250:ASN:HD22	2.23	0.46
2:B:629:ASN:HB3	2:B:642:HIS:CD2	2.45	0.46
2:D:572:ASN:HD22	2:D:573:LEU:N	2.13	0.46
2:D:651:SER:O	2:D:654:ASN:HB3	2.16	0.46
2:D:657:TYR:CG	2:D:658:ASP:N	2.83	0.46
2:D:598:LEU:HD11	2:F:599:LEU:HD13	1.98	0.46
2:B:628:ASN:ND2	2:B:659:TYR:HH	2.14	0.46
2:F:572:ASN:HD22	2:F:573:LEU:N	2.13	0.46
2:B:637:CYS:HB2	5:B:714:HOH:O	2.15	0.45
1:C:24:LEU:HD21	2:F:551:LYS:HE3	1.99	0.45
1:A:7:ILE:HG13	2:B:526:HIS:CB	2.46	0.45
1:A:224:ARG:NH2	3:G:1:NAG:O3	2.48	0.45
1:A:120:ILE:HG23	1:A:121:PHE:N	2.31	0.45
1:A:42:ASN:ND2	1:A:45:LYS:HB2	2.30	0.45
1:C:127:TRP:HZ3	1:C:164:LEU:HD13	1.80	0.45
1:E:37:LEU:HB2	1:E:315:LEU:HB2	1.97	0.45
1:E:115:PHE:CD1	1:E:115:PHE:C	2.95	0.45
1:A:158:GLY:O	1:A:159:SER:HB3	2.15	0.45
2:B:659:TYR:N	2:B:660:PRO:HD2	2.32	0.45
1:C:115:PHE:CD1	1:C:115:PHE:C	2.95	0.45
1:A:95:TYR:CD2	1:A:230:MET:HB2	2.51	0.45
2:D:650:GLU:O	2:D:654:ASN:CB	2.60	0.45
1:A:53:PRO:HB3	1:A:82:TYR:CZ	2.52	0.45
1:A:67:GLY:O	1:A:149:ARG:HG2	2.16	0.45
1:A:196:GLN:OE1	1:A:197:ASN:OD1	2.35	0.45
1:C:195:TYR:O	1:C:196:GLN:CB	2.65	0.45
1:C:192:GLN:O	1:C:196:GLN:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:659:TYR:CE2	2:D:661:LYS:CD	3.00	0.44
1:A:157:LYS:O	1:A:158:GLY:C	2.60	0.44
1:A:35:ASN:ND2	1:A:37:LEU:H	2.16	0.44
1:E:115:PHE:O	1:E:115:PHE:HD1	2.01	0.44
2:F:525:HIS:CD2	2:F:534:TYR:CE2	3.04	0.44
1:A:220:ARG:HE	1:C:210:ASN:CG	2.26	0.44
1:C:94:CYS:O	1:C:224:ARG:HD3	2.17	0.44
1:A:95:TYR:HD2	1:A:230:MET:HB2	1.83	0.44
2:B:634:GLY:C	2:B:636:GLY:H	2.25	0.44
1:C:180:TRP:HB3	1:C:254:PRO:HG3	2.00	0.44
1:A:9:ILE:HD13	2:B:619:TYR:HA	1.99	0.44
1:A:132(A):THR:HG22	1:A:133:LYS:H	1.83	0.44
2:F:633:ILE:HD11	2:F:639:GLU:HB2	2.00	0.44
2:D:652:VAL:C	2:D:654:ASN:H	2.26	0.43
2:D:641:TYR:CD1	2:D:664:GLU:HG3	2.52	0.43
1:E:35:ASN:ND2	1:E:37:LEU:H	2.16	0.43
1:E:63:GLY:CA	1:E:92:GLY:HA2	2.48	0.43
2:B:623:LYS:HB2	2:B:638:PHE:HZ	1.83	0.43
1:E:267:GLY:HA3	2:F:566:VAL:HG11	2.00	0.43
2:B:633:ILE:HD11	2:B:639:GLU:HB2	2.00	0.43
2:D:664:GLU:O	2:D:664:GLU:HG2	2.19	0.43
1:E:115:PHE:C	1:E:115:PHE:HD1	2.26	0.43
1:E:130:HIS:CE1	1:E:162:PRO:O	2.72	0.43
1:E:130:HIS:NE2	1:E:164:LEU:HB3	2.33	0.43
1:C:66:LEU:O	1:C:150:ASN:HB2	2.18	0.43
1:E:161:TYR:CB	1:E:195:TYR:O	2.67	0.43
1:A:299:HIS:HA	1:A:300:PRO:HD3	1.94	0.42
1:C:67:GLY:O	1:C:149:ARG:HG2	2.19	0.42
2:D:555:VAL:O	2:D:559:MET:HG2	2.19	0.42
2:B:526:HIS:CD2	2:B:649:MET:CG	2.88	0.42
1:A:294:PRO:HG3	2:B:556:ILE:HG12	2.00	0.42
2:B:572:ASN:HD22	2:B:573:LEU:N	2.17	0.42
2:B:645:ASP:O	2:B:646:ASP:C	2.63	0.42
1:C:115:PHE:C	1:C:115:PHE:HD1	2.28	0.42
1:C:327:ARG:HD2	1:C:327:ARG:O	2.19	0.42
1:E:7:ILE:HG23	1:E:7:ILE:O	2.20	0.42
2:B:668:LEU:C	2:B:670:ARG:H	2.27	0.42
2:D:530:GLN:NE2	2:D:645:ASP:HB2	2.35	0.42
2:B:528:ASN:ND2	2:B:529:GLU:N	2.63	0.42
1:E:164:LEU:HD12	1:E:164:LEU:C	2.45	0.42
2:D:625:GLN:HE22	2:D:655:GLY:HA2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:634:GLY:O	2:D:635:ASN:C	2.63	0.41
1:C:214:THR:HA	1:C:215:PRO:HD3	1.94	0.41
1:A:310:VAL:HG13	1:A:312:SER:N	2.32	0.41
1:A:267:GLY:HA3	2:B:566:VAL:HG11	2.03	0.41
1:C:8:CYS:O	2:D:524:TYR:HA	2.21	0.41
1:E:132(A):THR:HG22	1:E:133:LYS:N	2.34	0.41
1:E:317:MET:HE1	2:F:555:VAL:HG21	2.01	0.41
1:A:93:THR:O	1:A:93:THR:CG2	2.68	0.41
1:C:53:PRO:HB3	1:C:82:TYR:CZ	2.55	0.41
1:C:164:LEU:C	1:C:164:LEU:HD12	2.45	0.41
1:E:58:LYS:HA	1:E:88:ASN:O	2.20	0.41
1:E:130:HIS:HE1	1:E:162:PRO:O	2.04	0.41
2:F:555:VAL:O	2:F:559:MET:HG2	2.21	0.41
1:A:116:GLU:CD	1:A:174:LYS:HZ1	2.29	0.41
1:C:71:CYS:HB3	1:C:74:LEU:HD12	2.01	0.41
1:C:282:CYS:SG	1:C:289:ILE:HB	2.61	0.41
1:A:289:ILE:CD1	1:A:298:ILE:HD12	2.51	0.41
1:A:310:VAL:CG2	2:B:593:THR:HA	2.51	0.41
2:B:555:VAL:O	2:B:559:MET:HG2	2.21	0.41
1:E:85:GLU:O	1:E:270:THR:HA	2.21	0.40
1:E:222:LYS:HA	1:E:226:GLN:O	2.22	0.40
1:E:295:PHE:HE2	2:F:559:MET:HE2	1.85	0.40
2:F:602:LEU:HD12	2:F:602:LEU:HA	1.89	0.40
2:B:572:ASN:HD22	2:B:572:ASN:C	2.28	0.40
2:D:548:ILE:HD13	2:D:548:ILE:HA	1.91	0.40
1:A:63:GLY:CA	1:A:92:GLY:HA2	2.52	0.40
1:A:115:PHE:C	1:A:115:PHE:CD1	2.99	0.40
1:C:156:LYS:HD2	1:C:159:SER:HA	2.02	0.40
2:F:548:ILE:HD13	2:F:548:ILE:HA	1.96	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	322/324 (99%)	311 (97%)	10 (3%)	1 (0%)	36	66
1	C	322/324 (99%)	302 (94%)	19 (6%)	1 (0%)	36	66
1	E	322/324 (99%)	304 (94%)	16 (5%)	2 (1%)	21	51
2	B	168/170 (99%)	150 (89%)	14 (8%)	4 (2%)	4	17
2	D	162/170 (95%)	137 (85%)	17 (10%)	8 (5%)	1	6
2	F	163/170 (96%)	141 (86%)	16 (10%)	6 (4%)	2	9
All	All	1459/1482 (98%)	1345 (92%)	92 (6%)	22 (2%)	8	28

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	633	ILE
2	D	657	TYR
2	D	660	PRO
2	D	663	SER
1	E	125	SER
2	F	633	ILE
2	F	663	SER
1	A	158	GLY
1	C	125	SER
2	D	643	LYS
2	F	643	LYS
2	F	662	TYR
2	B	661	LYS
2	D	635	ASN
2	D	526	HIS
2	D	659	TYR
2	F	527	GLN
2	F	654	ASN
2	B	635	ASN
2	B	634	GLY
2	B	633	ILE
1	E	158	GLY

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	278/278 (100%)	257 (92%)	21 (8%)	12	36
1	C	278/278 (100%)	264 (95%)	14 (5%)	22	54
1	E	278/278 (100%)	261 (94%)	17 (6%)	17	46
2	B	145/145 (100%)	132 (91%)	13 (9%)	9	28
2	D	139/145 (96%)	127 (91%)	12 (9%)	10	31
2	F	140/145 (97%)	128 (91%)	12 (9%)	10	31
All	All	1258/1269 (99%)	1169 (93%)	89 (7%)	13	39

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	A	23	VAL
1	A	49	LEU
1	A	49(A)	LYS
1	A	58	LYS
1	A	90	GLU
1	A	93	THR
1	A	115	PHE
1	A	131	GLU
1	A	140	SER
1	A	151	LEU
1	A	152	LEU
1	A	171	ASN
1	A	174	LYS
1	A	199	ASP
1	A	214	THR
1	A	216	GLU
1	A	217	ILE
1	A	281	LYS
1	A	302	THR
1	A	310	VAL
2	B	519	ASP
2	B	522	TYR
2	B	528	ASN
2	B	572	ASN
2	B	575	ARG
2	B	580	LEU
2	B	598	LEU

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Mol	Chain	Res	Type
2	B	602	LEU
2	B	629	ASN
2	B	635	ASN
2	B	643	LYS
2	B	644	CYS
2	B	670	ARG
1	C	23	VAL
1	C	58	LYS
1	C	93	THR
1	C	115	PHE
1	C	131	GLU
1	C	151	LEU
1	C	152	LEU
1	C	190	ASP
1	C	266	SER
1	C	278	CYS
1	C	281	LYS
1	C	302	THR
1	C	310	VAL
1	C	321	LEU
2	D	519	ASP
2	D	526	HIS
2	D	527	GLN
2	D	572	ASN
2	D	575	ARG
2	D	580	LEU
2	D	598	LEU
2	D	602	LEU
2	D	659	TYR
2	D	661	LYS
2	D	662	TYR
2	D	663	SER
1	E	23	VAL
1	E	49	LEU
1	E	49(A)	LYS
1	E	55	GLN
1	E	58	LYS
1	E	90	GLU
1	E	93	THR
1	E	115	PHE
1	E	131	GLU
1	E	151	LEU

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Mol	Chain	Res	Type
1	E	152	LEU
1	E	189	THR
1	E	196	GLN
1	E	278	CYS
1	E	281	LYS
1	E	302	THR
1	E	310	VAL
2	F	519	ASP
2	F	526	HIS
2	F	527	GLN
2	F	540	SER
2	F	572	ASN
2	F	580	LEU
2	F	598	LEU
2	F	602	LEU
2	F	659	TYR
2	F	661	LYS
2	F	663	SER
2	F	664	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	35	ASN
1	A	171	ASN
1	A	191	GLN
1	A	250	ASN
2	B	528	ASN
2	B	530	GLN
2	B	562	GLN
2	B	572	ASN
2	B	625	GLN
2	B	629	ASN
1	C	35	ASN
1	C	42	ASN
1	C	191	GLN
1	C	196	GLN
1	C	250	ASN
2	D	526	HIS
2	D	530	GLN
2	D	562	GLN

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Mol	Chain	Res	Type
2	D	572	ASN
2	D	581	ASN
2	D	625	GLN
2	D	629	ASN
2	D	635	ASN
2	D	654	ASN
1	E	27	ASN
1	E	35	ASN
1	E	42	ASN
1	E	55	GLN
1	E	130	HIS
1	E	150	ASN
1	E	191	GLN
1	E	196	GLN
1	E	250	ASN
2	F	525	HIS
2	F	526	HIS
2	F	530	GLN
2	F	562	GLN
2	F	572	ASN
2	F	625	GLN
2	F	629	ASN
2	F	635	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 ⓘ

9 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	1,3	14,14,15	0.52	0	17,19,21	0.87	1 (5%)
3	NAG	G	2	3	14,14,15	0.47	0	17,19,21	0.78	0
4	NAG	H	1	4	14,14,15	0.56	0	17,19,21	0.68	0
4	GAL	H	2	4	11,11,12	0.68	0	15,15,17	1.32	2 (13%)
4	SIA	H	3	4	20,20,21	0.56	0	21,28,31	0.82	2 (9%)
3	NAG	I	1	1,3	14,14,15	0.51	0	17,19,21	0.94	1 (5%)
3	NAG	I	2	3	14,14,15	0.50	0	17,19,21	0.70	0
3	NAG	J	1	1,3	14,14,15	0.48	0	17,19,21	0.85	0
3	NAG	J	2	3	14,14,15	0.46	0	17,19,21	0.80	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
4	NAG	H	1	4	-	0/6/23/26	0/1/1/1
4	GAL	H	2	4	-	0/2/19/22	0/1/1/1
4	SIA	H	3	4	-	0/18/34/38	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	2	GAL	C1-C2-C3	3.77	115.13	109.64
3	I	1	NAG	C1-O5-C5	2.74	115.86	112.19
4	H	2	GAL	O3-C3-C2	-2.68	104.58	110.05
4	H	3	SIA	O1B-C1-C2	2.22	118.48	112.71
3	G	1	NAG	C3-C4-C5	-2.03	106.56	110.23
4	H	3	SIA	O1A-C1-C2	-2.01	118.50	122.85

There are no chirality outliers.

All (5) torsion outliers are listed below:

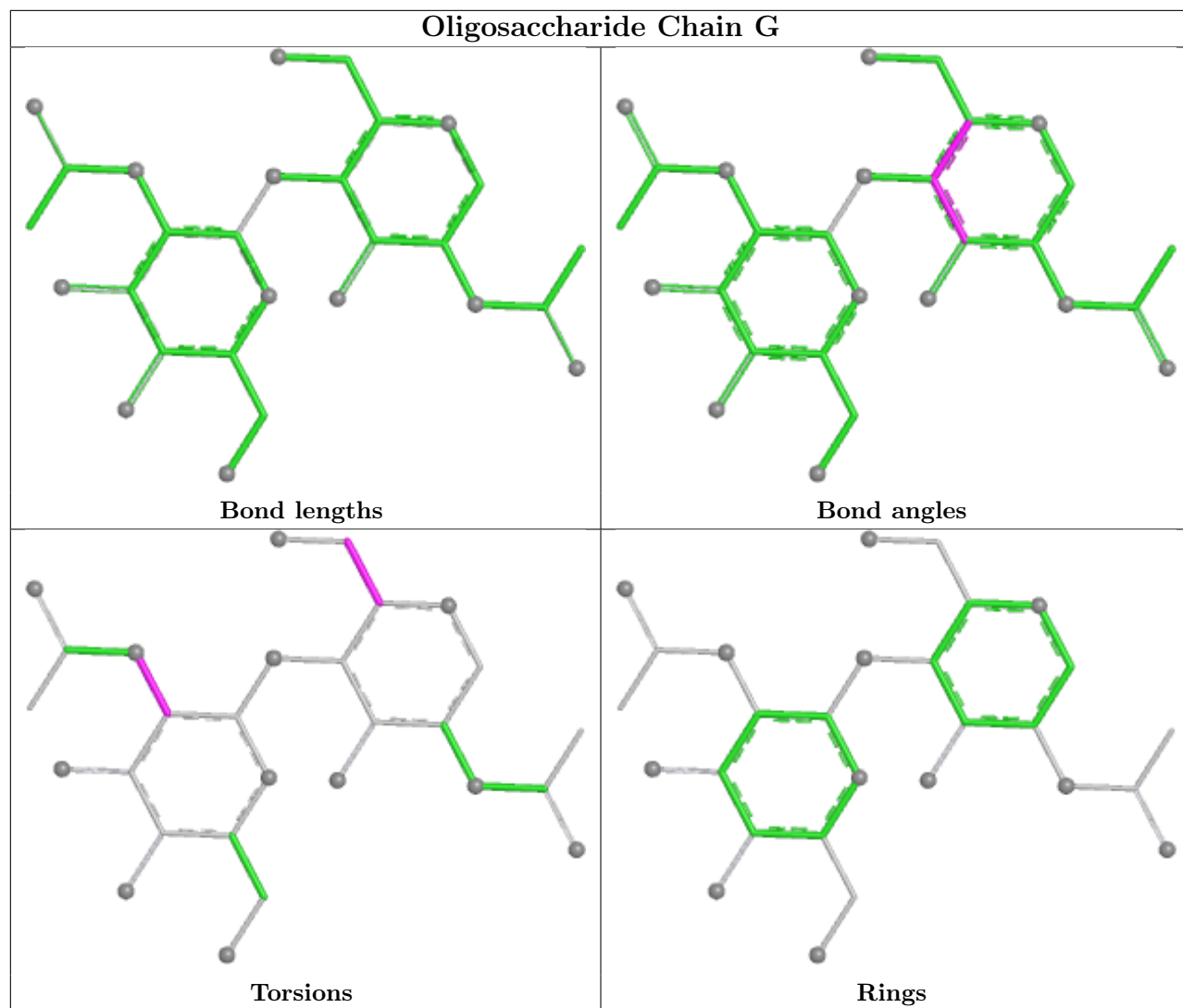
Mol	Chain	Res	Type	Atoms
3	G	1	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	G	2	NAG	C1-C2-N2-C7

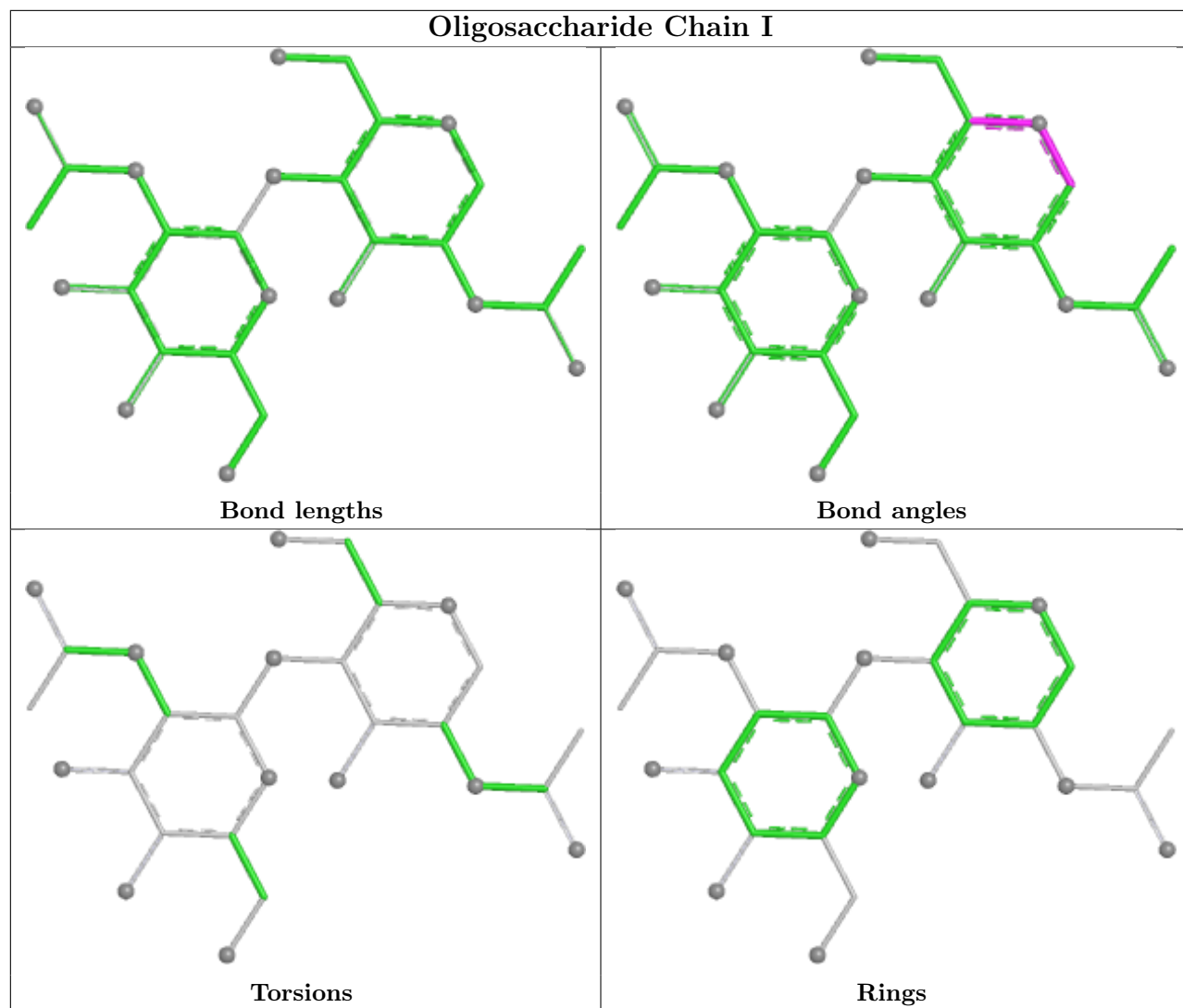
There are no ring outliers.

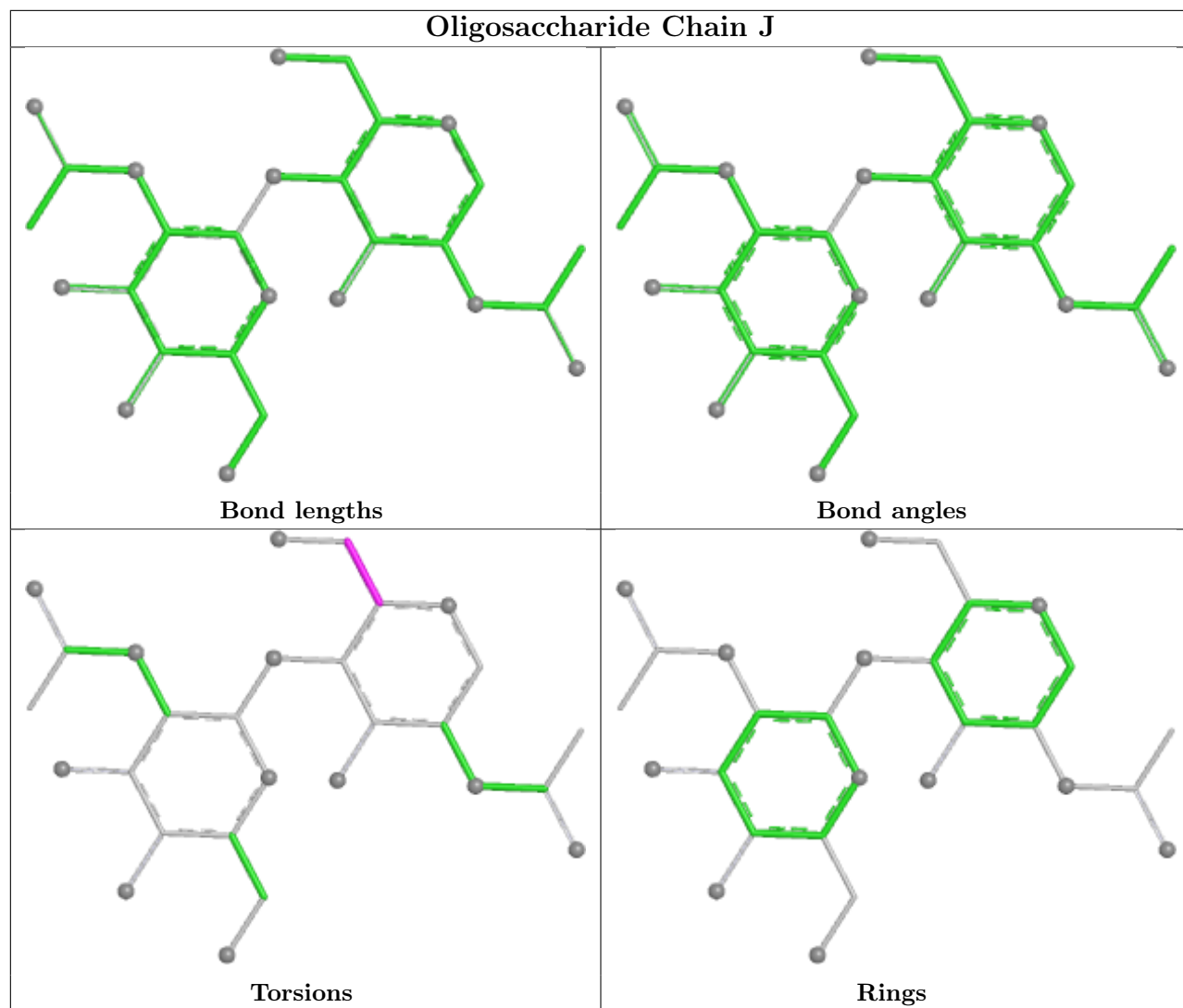
4 monomers are involved in 4 short contacts:

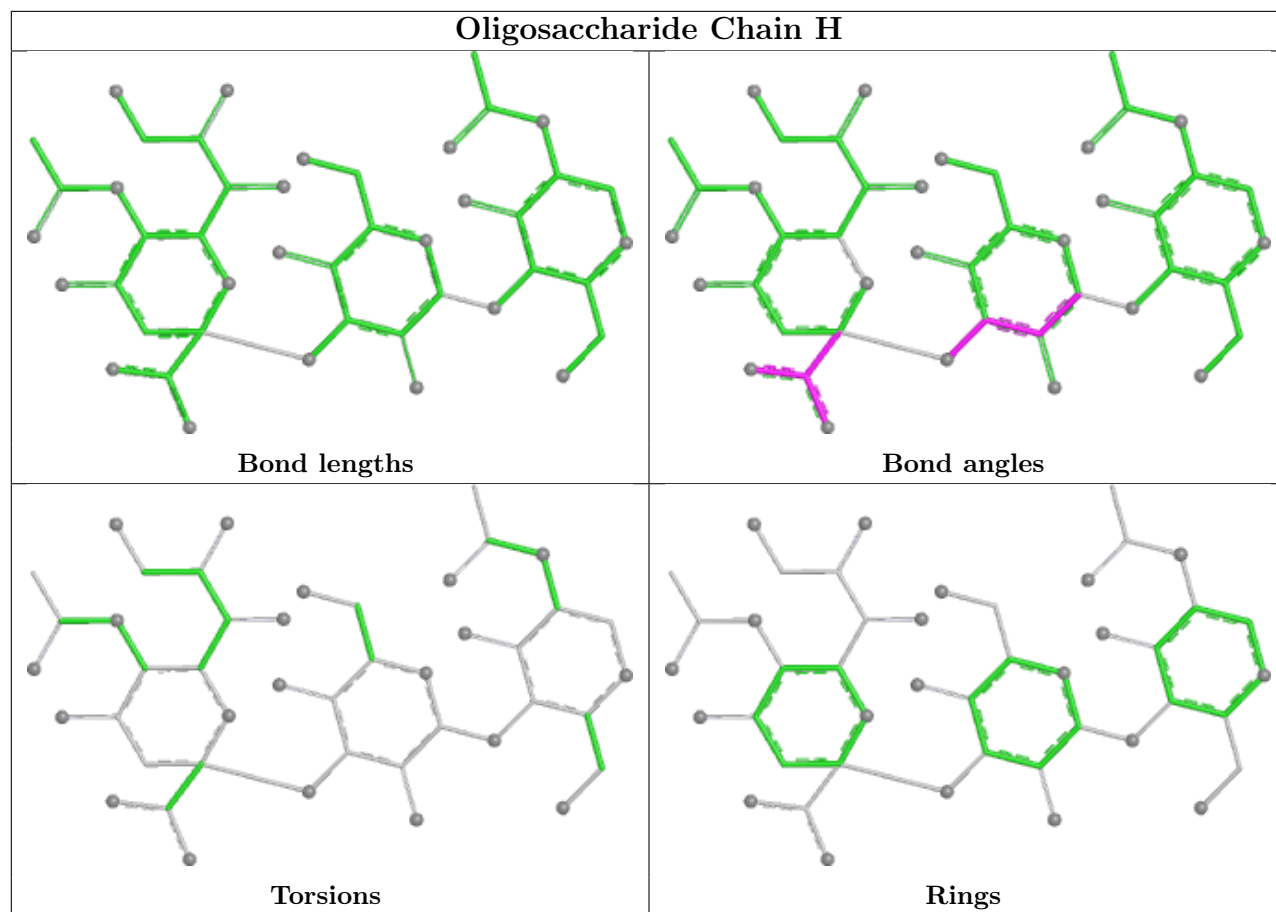
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	1	NAG	1	0
3	I	1	NAG	1	0
4	H	3	SIA	1	0
3	G	1	NAG	1	0

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









5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	324/324 (100%)	-0.25	3 (0%) 81 74	21, 42, 72, 178	0
1	C	324/324 (100%)	-0.16	5 (1%) 72 63	22, 50, 78, 188	0
1	E	324/324 (100%)	-0.28	7 (2%) 62 52	22, 43, 74, 165	0
2	B	170/170 (100%)	0.11	6 (3%) 47 38	30, 56, 85, 116	0
2	D	164/170 (96%)	0.44	14 (8%) 16 12	33, 69, 113, 144	0
2	F	165/170 (97%)	0.36	12 (7%) 21 15	31, 68, 118, 150	0
All	All	1471/1482 (99%)	-0.05	47 (3%) 50 40	21, 51, 97, 188	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	660	PRO	4.8
2	D	660	PRO	4.7
2	B	663	SER	4.2
2	B	526	HIS	3.9
1	E	326	ALA	3.7
2	D	560	ASN	3.5
1	C	132(A)	THR	3.3
2	B	562	GLN	3.2
1	E	42	ASN	3.2
2	D	643	LYS	3.1
1	A	199	ASP	3.1
1	E	5	ASP	3.0
2	F	561	THR	2.9
2	D	529	GLU	2.9
2	D	519	ASP	2.8
2	D	663	SER	2.8
2	F	664	GLU	2.7
2	D	659	TYR	2.7
2	F	657	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
2	F	643	LYS	2.7
1	C	277	ASP	2.7
2	F	519	ASP	2.7
2	B	665	GLU	2.7
2	D	559	MET	2.6
1	E	327	ARG	2.6
2	B	567	GLY	2.6
1	C	326	ALA	2.6
2	D	501	GLY	2.4
2	B	561	THR	2.3
2	F	659	TYR	2.3
2	F	665	GLU	2.3
2	F	621	LYS	2.2
1	A	326	ALA	2.2
2	D	628	ASN	2.2
2	D	642	HIS	2.2
1	E	276	HIS	2.2
1	E	44	GLY	2.2
2	F	538	GLN	2.1
1	C	219	ALA	2.1
1	E	278	CYS	2.1
1	A	5	ASP	2.1
2	F	640	PHE	2.1
2	F	560	ASN	2.1
2	D	664	GLU	2.1
1	C	55	GLN	2.0
2	D	528	ASN	2.0
2	D	548	ILE	2.0

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

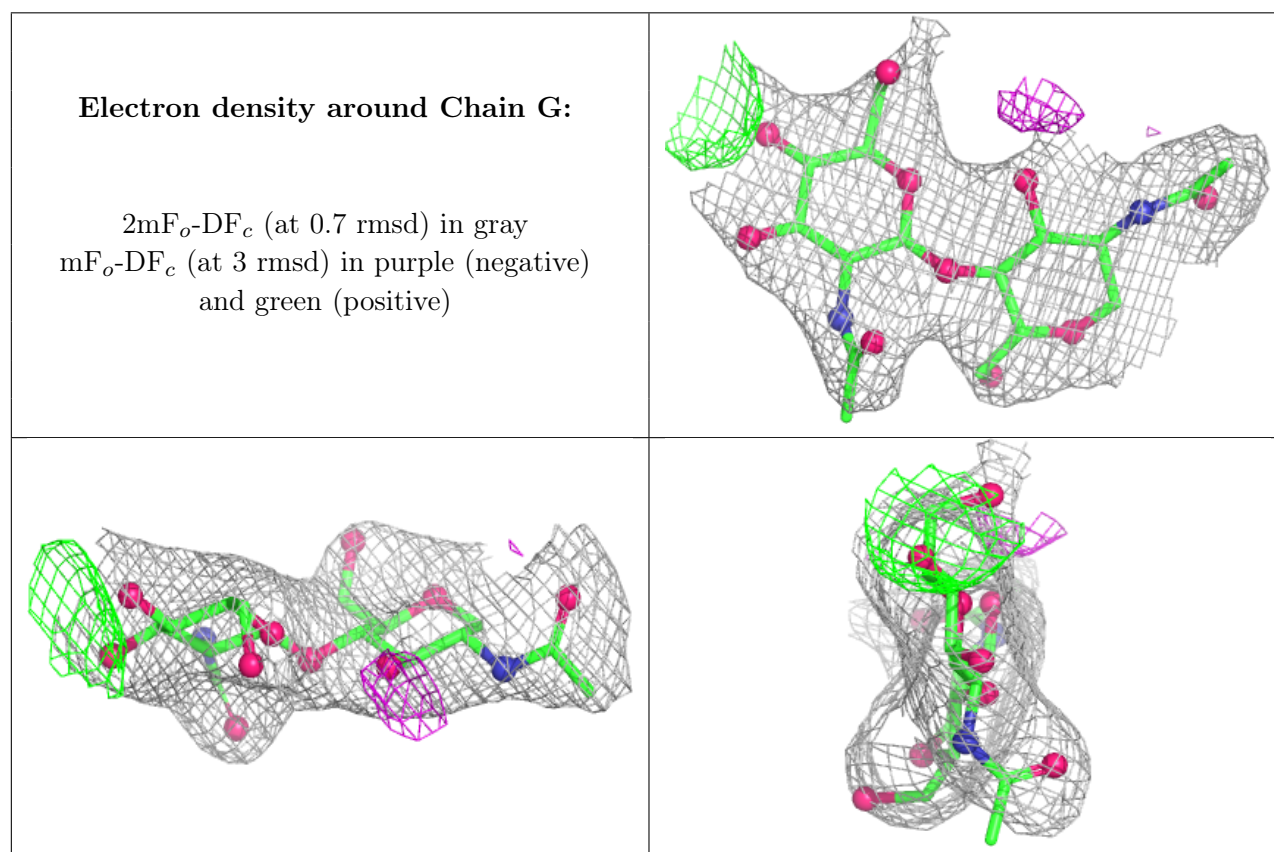
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

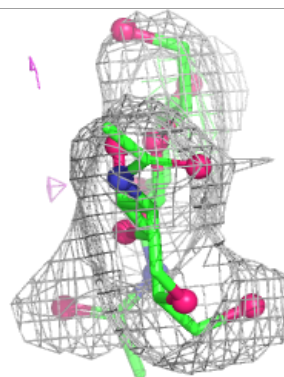
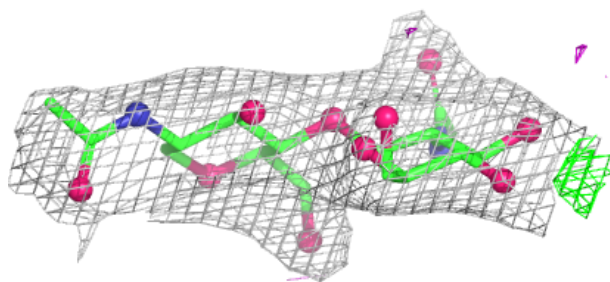
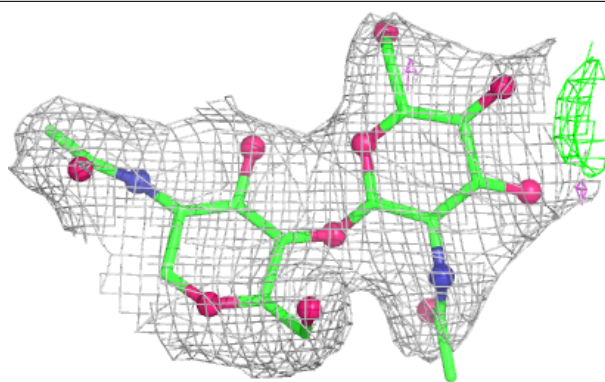
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	H	1	14/15	0.64	0.17	72,87,110,113	0
3	NAG	I	2	14/15	0.85	0.12	67,73,82,82	0
3	NAG	J	2	14/15	0.88	0.12	70,78,89,90	0
3	NAG	G	2	14/15	0.88	0.10	52,63,74,76	0
4	GAL	H	2	11/12	0.89	0.09	36,46,54,58	0
4	SIA	H	3	20/21	0.93	0.09	38,41,46,49	0
3	NAG	I	1	14/15	0.94	0.08	42,47,53,55	0
3	NAG	G	1	14/15	0.94	0.09	32,41,59,64	0
3	NAG	J	1	14/15	0.96	0.06	35,44,49,53	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.

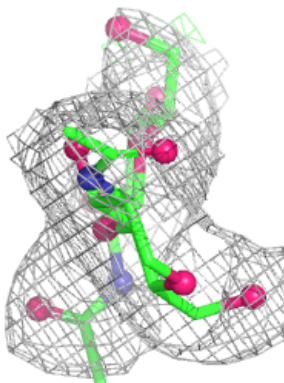
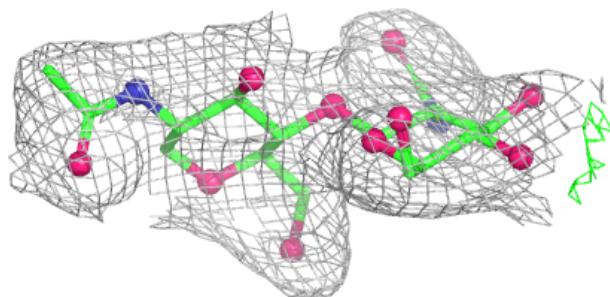
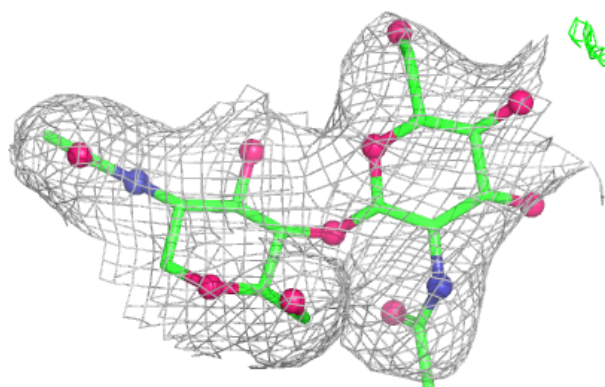


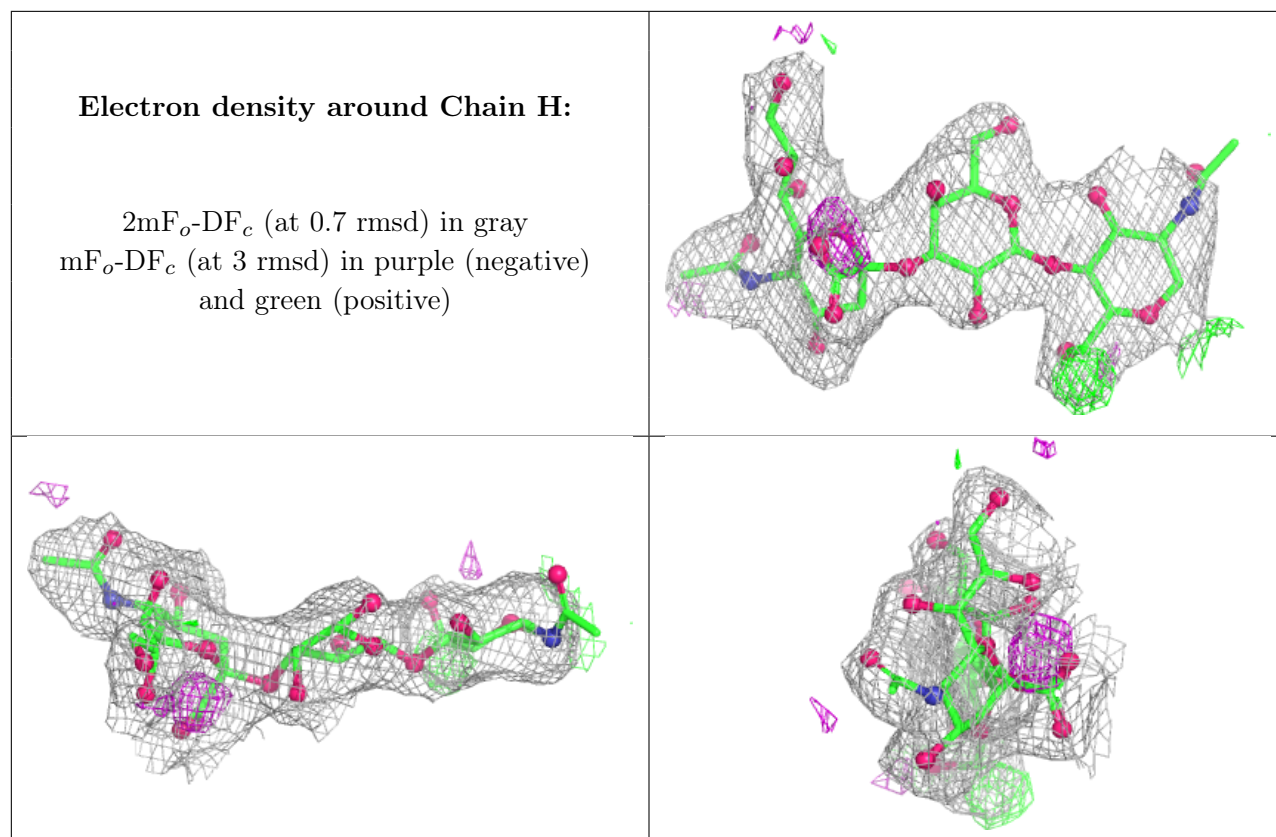
Electron density around Chain I:

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

**Electron density around Chain J:**

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





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.