



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:05 AM UTC

PDB ID : 6D8D / pdb_00006d8d
Title : The crystal structure of hemagglutinin from A/Hong Kong/125/2017 influenza virus in complex with LSTb
Authors : Yang, H.; Stevens, J.
Deposited on : 2018-04-26
Resolution : 3.55 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:

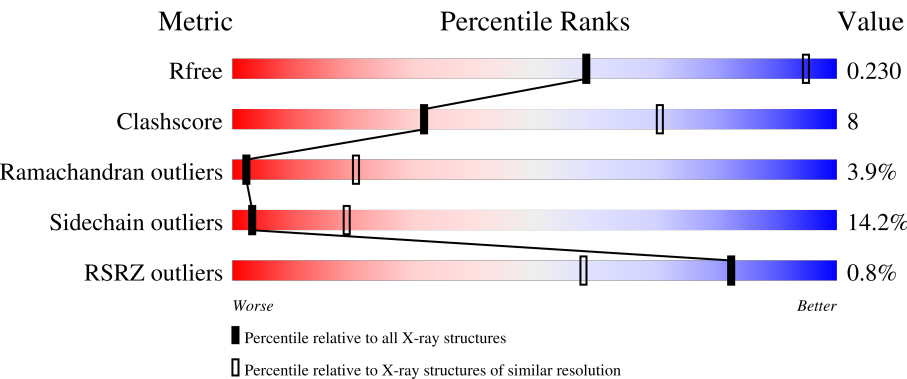
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 3.55 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	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)

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	321	64%29%5% ..
1	C	321	% 64%28%6% ..
1	E	321	% 64%28%5% ..
2	B	221	53%20%.23%
2	D	221	% 51%23%.23%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	221	% 52%21%23%
3	G	3	100%
3	H	3	100%
4	I	2	100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11670 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.

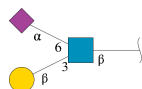
- Molecule 1 is a protein called Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	1	0	0
			2416	1503	435	464	14			
1	C	316	Total	C	N	O	S	1	0	0
			2416	1503	435	464	14			
1	E	316	Total	C	N	O	S	1	0	0
			2416	1503	435	464	14			

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	171	Total	C	N	O	S	0	0	0
			1389	859	245	278	7			
2	D	171	Total	C	N	O	S	0	0	0
			1389	859	245	278	7			
2	F	171	Total	C	N	O	S	0	0	0
			1389	859	245	278	7			

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



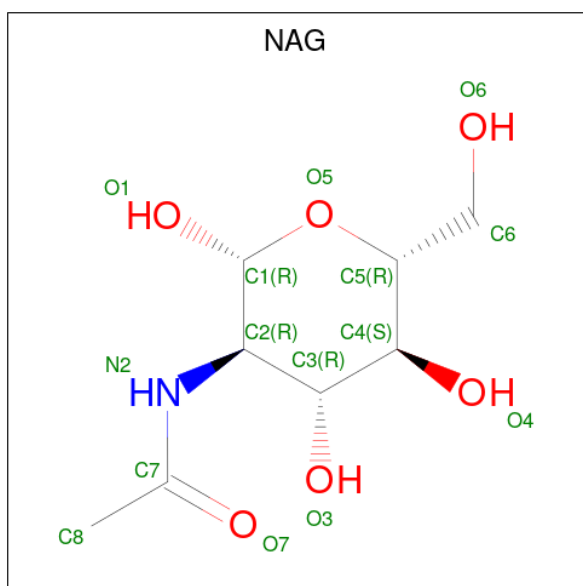
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	3	Total	C	N	O	0	0	0
			45	25	2	18			
3	H	3	Total	C	N	O	0	0	0
			45	25	2	18			

- Molecule 4 is an oligosaccharide called beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



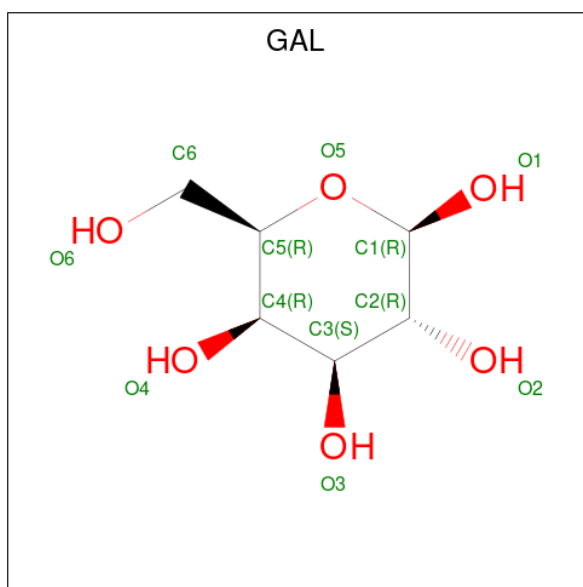
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	2	Total	C	N	O	0	0	0
			25	14	1	10			

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



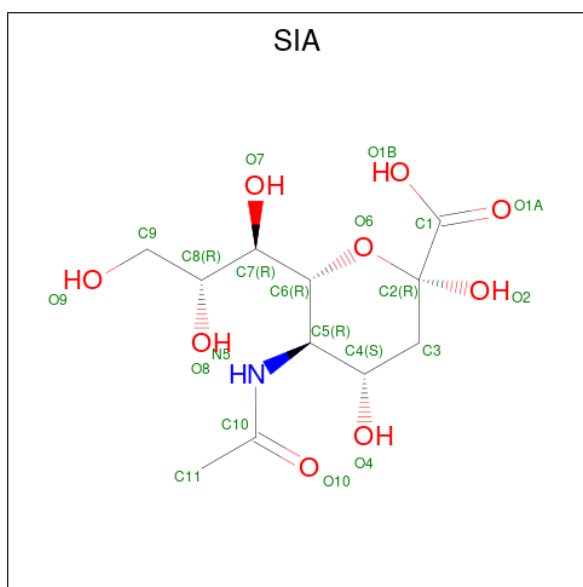
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is beta-D-galactopyranose (CCD ID: GAL) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			12	6	6		
6	C	1	Total	C	O	0	0
			12	6	6		
6	E	1	Total	C	O	0	0
			12	6	6		

- Molecule 7 is N-acetyl-alpha-neuraminic acid (CCD ID: SIA) (formula: $C_{11}H_{19}NO_9$).

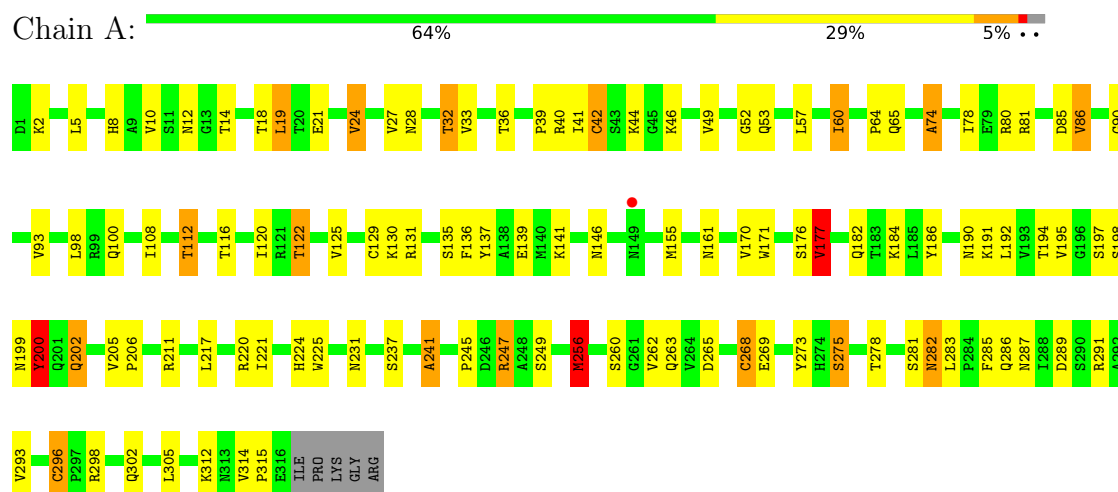


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	1	Total	C	N	O	0	0
			20	11	1	8		

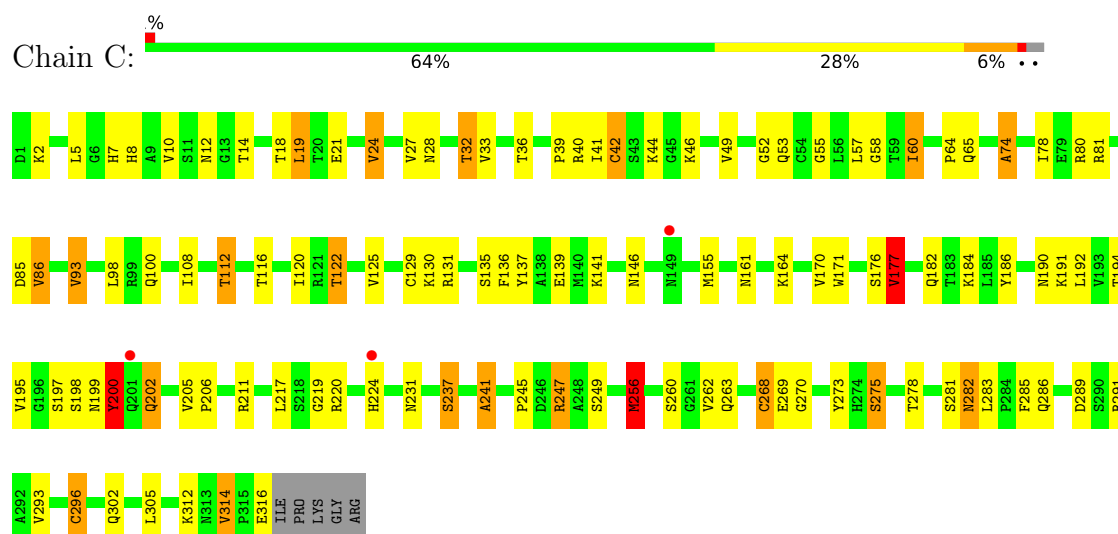
3 Residue-property plots

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 HA1 chain

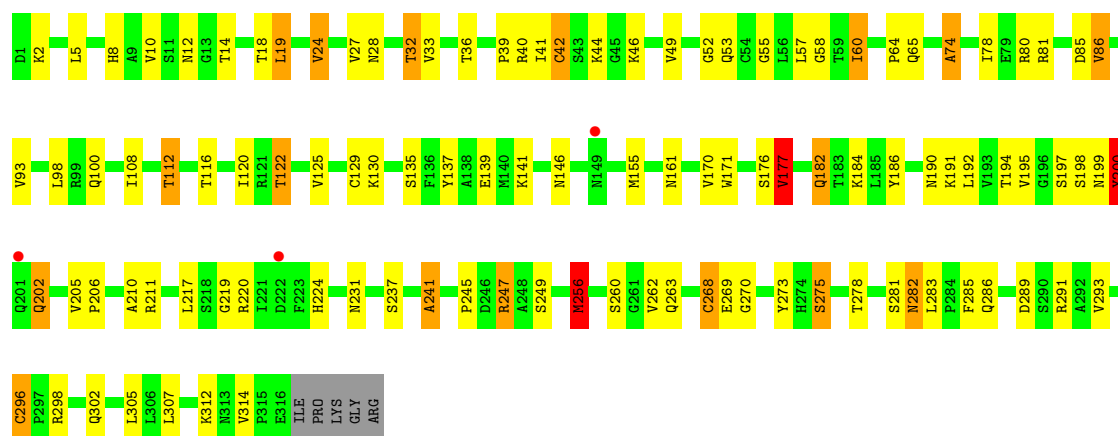


• Molecule 1: Hemagglutinin HA1 chain



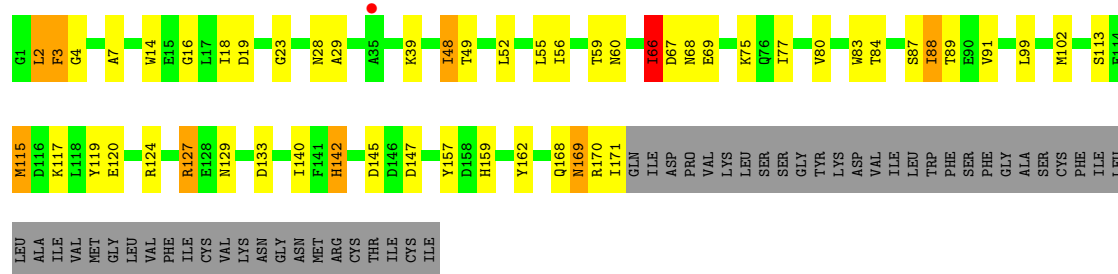
• Molecule 1: Hemagglutinin HA1 chain





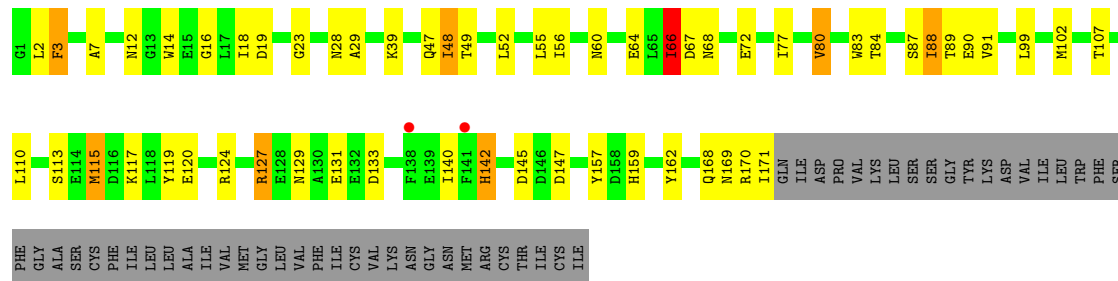
• Molecule 2: Hemagglutinin HA2 chain

Chain B: 53% 20% • 23%



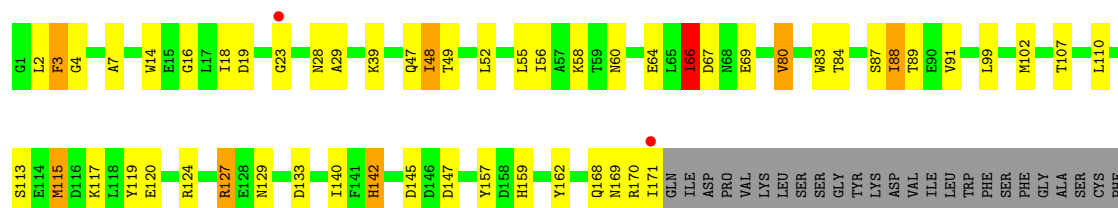
• Molecule 2: Hemagglutinin HA2 chain

Chain D: 51% 23% • 23%



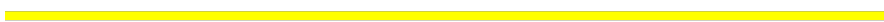
• Molecule 2: Hemagglutinin HA2 chain

Chain F: 52% 21% • 23%



ILE
LEU
LEU
ALA
ILE
VAL
MET
GLY
LEU
VAL
PHE
ILE
CYS
VAL
LYS
ASN
GLY
ASN
MET
ARG
CYS
THR
ILE
CYS
ILE

- Molecule 3: beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%

MAG1
GAL2
SIA3

- Molecule 3: beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%

MAG1
GAL2
SIA3

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

Chain I:  100%

MAG1
GAL2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	203.57Å 117.87Å 119.86Å 90.00° 124.21° 90.00°	Depositor
Resolution (Å)	50.01 – 3.55 50.01 – 3.55	Depositor EDS
% Data completeness (in resolution range)	91.9 (50.01-3.55) 91.9 (50.01-3.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.221 , 0.260 (Not available) , 0.230	Depositor DCC
R_{free} test set	1297 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for $1/2^*h+1/2^*k+2^*l, 1/2^*h+1/2^*k, -1/2^*h+1/2^*k-l$ 0.000 for $-1/2^*h-3/2^*k-l, -1/2^*h+1/2^*k-l, 1/2^*h+1/2^*k$ 0.000 for $-1/2^*h+3/2^*k-l, 1/2^*h+1/2^*k+l, 1/2^*h-1/2^*k$ 0.000 for $1/2^*h-1/2^*k+2^*l, -1/2^*h+1/2^*k, -1/2^*h-1/2^*k-l$ 0.000 for $-h+k-l, -l, -k$ 0.000 for $-h-k-l, l, k$ 0.000 for $-1/2^*h+1/2^*k+l, 1/2^*h-1/2^*k+l, 1/2^*h+1/2^*k$ 0.000 for $-1/2^*h-1/2^*k+l, -1/2^*h-1/2^*k-l, 1/2^*h-1/2^*k$ 0.398 for $1/2^*h+3/2^*k, 1/2^*h-1/2^*k, -1/2^*h-1/2^*k-l$ 0.390 for $1/2^*h-3/2^*k, -1/2^*h-1/2^*k, -1/2^*h+1/2^*k-l$ 0.000 for $-h-2^*l, -k, l$	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11670	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

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.

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

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: GAL, SIA, 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	1.16	6/2462 (0.2%)	1.23	11/3329 (0.3%)
1	C	1.16	5/2462 (0.2%)	1.24	11/3329 (0.3%)
1	E	1.16	6/2462 (0.2%)	1.23	11/3329 (0.3%)
2	B	1.13	1/1413 (0.1%)	1.26	9/1903 (0.5%)
2	D	1.14	1/1413 (0.1%)	1.26	12/1903 (0.6%)
2	F	1.14	1/1413 (0.1%)	1.26	10/1903 (0.5%)
All	All	1.15	20/11625 (0.2%)	1.24	64/15696 (0.4%)

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
1	C	0	1
1	E	0	1
2	B	0	1
2	D	0	1
2	F	0	1
All	All	0	6

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	268	CYS	CB-SG	-6.97	1.58	1.81
2	F	66	ILE	N-CA	6.84	1.53	1.46
2	D	66	ILE	N-CA	6.30	1.52	1.46
2	B	66	ILE	N-CA	6.15	1.52	1.46
1	E	177	VAL	CA-C	5.82	1.60	1.52
1	C	268	CYS	CB-SG	-5.81	1.62	1.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	177	VAL	CA-C	5.75	1.60	1.52
1	C	100	GLN	CA-C	5.64	1.60	1.52
1	C	177	VAL	CA-C	5.60	1.59	1.52
1	A	100	GLN	CA-C	5.49	1.59	1.52
1	E	286	GLN	CA-C	-5.43	1.46	1.52
1	C	28	ASN	CA-CB	5.42	1.61	1.53
1	E	100	GLN	CA-C	5.39	1.59	1.52
1	E	28	ASN	CA-CB	5.35	1.61	1.53
1	A	268	CYS	CB-SG	-5.33	1.63	1.81
1	E	177	VAL	CA-CB	5.31	1.61	1.54
1	A	286	GLN	CA-C	-5.29	1.46	1.52
1	C	286	GLN	CA-C	-5.25	1.46	1.52
1	A	28	ASN	CA-CB	5.21	1.61	1.53
1	A	177	VAL	CA-CB	5.14	1.61	1.54

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	74	ALA	N-CA-C	7.77	120.67	108.79
1	A	74	ALA	N-CA-C	7.73	120.61	108.79
1	C	74	ALA	N-CA-C	7.60	120.42	108.79
1	C	289	ASP	N-CA-C	-7.45	96.28	108.41
1	A	289	ASP	N-CA-C	-7.31	96.50	108.41
1	E	289	ASP	N-CA-C	-7.07	96.88	108.41
2	F	88	ILE	N-CA-C	6.84	116.97	110.74
2	B	88	ILE	N-CA-C	6.71	116.84	110.74
2	D	88	ILE	N-CA-C	6.62	116.76	110.74
2	B	80	VAL	CB-CA-C	-6.10	103.80	112.22
2	D	80	VAL	CB-CA-C	-6.09	103.81	112.22
2	F	80	VAL	CB-CA-C	-6.09	103.82	112.22
2	F	14	TRP	N-CA-C	5.94	119.32	107.62
1	C	60	ILE	CB-CA-C	-5.91	104.75	111.55
1	C	256	MET	N-CA-C	-5.82	99.75	109.24
1	E	256	MET	N-CA-C	-5.82	99.76	109.24
1	A	296	CYS	CA-C-N	-5.78	114.80	120.98
1	A	296	CYS	C-N-CA	-5.78	114.80	120.98
1	A	24	VAL	N-CA-CB	5.77	116.82	110.53
1	A	256	MET	N-CA-C	-5.75	99.86	109.24
1	A	2	LYS	N-CA-C	5.74	116.13	108.38
1	E	60	ILE	CB-CA-C	-5.73	104.96	111.55
1	A	60	ILE	CB-CA-C	-5.72	104.97	111.55
1	E	296	CYS	CA-C-N	-5.69	114.89	120.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	296	CYS	C-N-CA	-5.69	114.89	120.98
2	F	84	THR	N-CA-C	-5.69	105.08	111.28
1	C	268	CYS	CA-CB-SG	5.67	127.43	114.40
1	E	268	CYS	CA-CB-SG	5.67	127.43	114.40
2	D	84	THR	N-CA-C	-5.64	105.14	111.28
1	C	2	LYS	N-CA-C	5.63	115.98	108.38
2	B	14	TRP	N-CA-C	5.63	118.72	107.62
2	D	14	TRP	N-CA-C	5.63	118.71	107.62
2	B	84	THR	N-CA-C	-5.59	105.19	111.28
1	C	112	THR	N-CA-CB	5.56	118.74	110.29
1	C	296	CYS	CA-C-N	-5.51	115.09	120.98
1	C	296	CYS	C-N-CA	-5.51	115.09	120.98
1	A	112	THR	N-CA-CB	5.46	118.59	110.29
1	C	24	VAL	N-CA-CB	5.46	116.67	110.72
2	D	67	ASP	N-CA-CB	-5.45	102.76	111.43
1	E	24	VAL	N-CA-CB	5.40	116.60	110.72
1	E	112	THR	N-CA-CB	5.37	118.46	110.29
2	F	48	ILE	N-CA-C	-5.36	105.10	110.30
2	F	67	ASP	N-CA-CB	-5.35	102.93	111.43
2	D	48	ILE	N-CA-C	-5.31	105.15	110.30
1	A	247	ARG	N-CA-C	5.29	118.07	109.24
2	B	23	GLY	N-CA-C	5.26	118.26	110.42
2	B	48	ILE	N-CA-C	-5.25	105.20	110.30
2	B	67	ASP	N-CA-CB	-5.23	103.12	111.43
2	D	23	GLY	N-CA-C	5.22	118.19	110.42
2	B	68	ASN	N-CA-C	5.19	116.49	107.93
2	D	68	ASN	N-CA-C	5.17	116.45	107.93
1	C	247	ARG	N-CA-C	5.15	117.84	109.24
2	F	23	GLY	N-CA-C	5.13	118.07	110.42
1	E	2	LYS	N-CA-C	5.07	115.22	108.38
2	B	66	ILE	CB-CA-C	-5.04	105.50	111.65
2	D	107	THR	CA-C-N	5.04	126.87	120.72
2	D	107	THR	C-N-CA	5.04	126.87	120.72
2	D	66	ILE	CB-CA-C	-5.04	105.50	111.65
1	E	247	ARG	N-CA-C	5.02	117.62	109.24
2	D	131	GLU	N-CA-C	5.01	117.41	109.50
2	F	107	THR	CA-C-N	5.01	126.83	120.72
2	F	107	THR	C-N-CA	5.01	126.83	120.72
1	A	225	TRP	N-CA-C	5.01	116.67	108.76
2	F	66	ILE	CB-CA-C	-5.00	105.55	111.65

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	THR	Peptide
2	B	66	ILE	Peptide
1	C	122	THR	Peptide
2	D	66	ILE	Peptide
1	E	122	THR	Peptide
2	F	66	ILE	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	2416	0	2382	41	0
1	C	2416	0	2382	48	0
1	E	2416	0	2382	44	0
2	B	1389	0	1300	26	0
2	D	1389	0	1300	28	0
2	F	1389	0	1300	30	0
3	G	45	0	38	0	0
3	H	45	0	38	0	0
4	I	25	0	20	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
5	C	14	0	13	1	0
5	D	14	0	13	0	0
5	E	14	0	13	0	0
5	F	14	0	13	0	0
6	A	12	0	12	0	0
6	C	12	0	12	0	0
6	E	12	0	12	0	0
7	E	20	0	17	0	0
All	All	11670	0	11273	185	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 (185) 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:256:MET:HA	1:A:256:MET:HE3	1.69	0.74
1:E:256:MET:HA	1:E:256:MET:HE3	1.69	0.73
1:C:256:MET:HE3	1:C:256:MET:HA	1.69	0.73
1:E:139:GLU:OE1	1:E:247:ARG:HD3	1.93	0.69
1:A:139:GLU:OE1	1:A:247:ARG:HD3	1.93	0.68
1:C:139:GLU:OE1	1:C:247:ARG:HD3	1.92	0.68
2:F:3:PHE:CD1	2:F:113:SER:HA	2.31	0.66
2:D:3:PHE:CD1	2:D:113:SER:HA	2.31	0.66
2:B:3:PHE:CD1	2:B:113:SER:HA	2.31	0.65
2:D:120:GLU:O	2:D:124:ARG:NH1	2.31	0.64
2:B:120:GLU:O	2:B:124:ARG:NH1	2.31	0.63
1:C:86:VAL:HG22	1:C:137:TYR:OH	1.98	0.63
1:C:19:LEU:HD13	2:D:102:MET:HA	1.80	0.63
2:F:120:GLU:O	2:F:124:ARG:NH1	2.31	0.63
1:E:42:CYS:HB2	1:E:278:THR:HG21	1.80	0.63
1:C:42:CYS:HB2	1:C:278:THR:HG21	1.81	0.62
1:E:86:VAL:HG22	1:E:137:TYR:OH	1.99	0.62
1:A:46:LYS:NZ	1:A:273:TYR:OH	2.32	0.62
1:A:86:VAL:HG22	1:A:137:TYR:OH	1.99	0.62
1:C:46:LYS:NZ	1:C:273:TYR:OH	2.34	0.61
1:A:42:CYS:HB2	1:A:278:THR:HG21	1.82	0.60
1:A:32:THR:HG22	1:A:305:LEU:HB2	1.84	0.60
1:E:46:LYS:NZ	1:E:273:TYR:OH	2.34	0.59
1:E:32:THR:HG22	1:E:305:LEU:HB2	1.85	0.58
1:C:32:THR:HG22	1:C:305:LEU:HB2	1.85	0.58
1:A:19:LEU:HD21	2:F:102:MET:CE	2.34	0.58
2:B:83:TRP:CD2	2:F:66:ILE:CD1	2.88	0.57
1:E:197:SER:OG	1:E:198:SER:N	2.38	0.57
2:F:127:ARG:HG3	2:F:159:HIS:CG	2.40	0.57
2:D:127:ARG:HG3	2:D:159:HIS:CG	2.40	0.56
1:A:197:SER:OG	1:A:198:SER:N	2.38	0.56
1:C:197:SER:OG	1:C:198:SER:N	2.38	0.56
2:B:127:ARG:HG3	2:B:159:HIS:CG	2.40	0.56
1:C:57:LEU:HD22	1:C:98:LEU:HD23	1.88	0.56
1:A:57:LEU:HD22	1:A:98:LEU:HD23	1.88	0.56
1:E:302:GLN:HG2	1:E:305:LEU:HD21	1.88	0.55
1:A:19:LEU:HD13	2:B:102:MET:HA	1.87	0.55
2:D:66:ILE:CD1	2:F:83:TRP:CD2	2.90	0.55
1:A:302:GLN:HG2	1:A:305:LEU:HD21	1.89	0.55
1:C:52:GLY:HA2	1:C:80:ARG:HG3	1.89	0.55
1:E:57:LEU:HD22	1:E:98:LEU:HD23	1.89	0.55
2:B:66:ILE:CD1	2:D:83:TRP:CD2	2.90	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:LYS:HB3	1:E:269:GLU:HB2	1.88	0.54
1:C:302:GLN:HG2	1:C:305:LEU:HD21	1.88	0.54
2:D:28:ASN:HD22	2:D:145:ASP:HA	1.73	0.54
1:E:52:GLY:HA2	1:E:80:ARG:HG3	1.89	0.54
1:C:182:GLN:HE22	1:C:206:PRO:HG2	1.73	0.54
1:A:182:GLN:HE22	1:A:206:PRO:HG2	1.73	0.54
2:B:28:ASN:HD22	2:B:145:ASP:HA	1.73	0.54
1:A:192:LEU:HD12	1:A:205:VAL:HG22	1.90	0.53
1:E:192:LEU:HD12	1:E:205:VAL:HG22	1.91	0.53
1:A:52:GLY:HA2	1:A:80:ARG:HG3	1.90	0.53
1:A:282:ASN:HB2	2:B:56:ILE:HG23	1.90	0.53
1:A:44:LYS:HB3	1:A:269:GLU:HB2	1.92	0.52
1:C:192:LEU:HD12	1:C:205:VAL:HG22	1.91	0.52
2:F:28:ASN:HD22	2:F:145:ASP:HA	1.73	0.52
1:E:19:LEU:HD13	2:F:102:MET:HA	1.90	0.52
1:C:120:ILE:HG12	1:C:155:MET:HE1	1.92	0.51
2:B:102:MET:CE	1:C:19:LEU:HD21	2.41	0.51
2:B:16:GLY:O	2:B:18:ILE:HG23	2.11	0.51
1:C:44:LYS:HB3	1:C:269:GLU:HB2	1.92	0.51
1:A:120:ILE:HG12	1:A:155:MET:HE1	1.92	0.51
2:D:16:GLY:O	2:D:18:ILE:HG23	2.11	0.51
2:D:115:MET:HE3	2:D:115:MET:HA	1.93	0.51
1:E:186:TYR:CZ	1:E:241:ALA:HA	2.46	0.50
2:F:16:GLY:O	2:F:18:ILE:HG23	2.11	0.50
2:B:77:ILE:HD11	2:D:80:VAL:HG21	1.94	0.50
1:C:5:LEU:HD23	2:D:119:TYR:HD1	1.76	0.50
1:E:120:ILE:HG12	1:E:155:MET:HE1	1.92	0.50
1:C:186:TYR:CZ	1:C:241:ALA:HA	2.46	0.50
2:F:115:MET:HE3	2:F:115:MET:HA	1.92	0.50
1:E:191:LYS:O	1:E:206:PRO:HD2	2.12	0.50
1:A:191:LYS:O	1:A:206:PRO:HD2	2.12	0.50
1:A:186:TYR:CZ	1:A:241:ALA:HA	2.46	0.49
1:A:49:VAL:HG23	1:A:74:ALA:HB2	1.95	0.49
1:A:211:ARG:HD2	1:A:220:ARG:HG2	1.93	0.49
2:B:115:MET:HE3	2:B:115:MET:HA	1.93	0.49
1:C:191:LYS:O	1:C:206:PRO:HD2	2.13	0.49
1:C:256:MET:HE1	2:D:64:GLU:HG2	1.94	0.49
1:C:211:ARG:HD2	1:C:220:ARG:HG2	1.94	0.48
1:E:5:LEU:HD23	2:F:119:TYR:HD1	1.77	0.48
1:C:282:ASN:HB2	2:D:56:ILE:HG23	1.94	0.48
1:C:46:LYS:NZ	1:C:270:GLY:O	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:211:ARG:HD2	1:E:220:ARG:HG2	1.94	0.48
1:A:5:LEU:HD23	2:B:119:TYR:HD1	1.78	0.48
1:E:293:VAL:O	1:E:296:CYS:SG	2.72	0.48
2:D:102:MET:HE3	1:E:19:LEU:HD21	1.96	0.47
1:E:49:VAL:HG23	1:E:74:ALA:HB2	1.95	0.47
1:C:19:LEU:HD13	2:D:102:MET:CA	2.44	0.47
1:C:49:VAL:HG23	1:C:74:ALA:HB2	1.96	0.47
1:A:60:ILE:HG21	1:A:170:VAL:HG21	1.97	0.47
1:C:293:VAL:O	1:C:296:CYS:SG	2.72	0.47
1:A:293:VAL:O	1:A:296:CYS:SG	2.73	0.46
1:A:195:VAL:HG12	1:A:200:TYR:HE2	1.79	0.46
1:E:195:VAL:HG12	1:E:200:TYR:HE2	1.80	0.46
1:A:170:VAL:O	1:A:245:PRO:HB3	2.16	0.46
1:A:281:SER:OG	1:A:283:LEU:HG	2.16	0.46
2:F:55:LEU:HD22	2:F:99:LEU:HD21	1.98	0.46
1:C:195:VAL:HG12	1:C:200:TYR:HE2	1.80	0.46
1:A:39:PRO:O	1:A:40:ARG:HG3	2.16	0.46
1:E:256:MET:HE1	2:F:64:GLU:HG2	1.97	0.45
1:E:281:SER:OG	1:E:283:LEU:HG	2.16	0.45
1:C:7:HIS:HE1	1:C:314:VAL:HG23	1.82	0.45
1:C:60:ILE:HG21	1:C:170:VAL:HG21	1.98	0.45
1:C:171:TRP:CE2	1:C:224:HIS:HB2	2.52	0.45
1:E:211:ARG:HD2	1:E:220:ARG:CG	2.47	0.45
1:C:39:PRO:O	1:C:40:ARG:HG3	2.16	0.45
1:C:41:ILE:HG21	1:C:78:ILE:HD11	1.99	0.45
1:E:170:VAL:O	1:E:245:PRO:HB3	2.16	0.45
1:C:49:VAL:CG2	1:C:74:ALA:HB2	2.47	0.45
1:A:211:ARG:HD2	1:A:220:ARG:CG	2.47	0.45
2:D:168:GLN:O	2:D:171:ILE:N	2.50	0.45
1:C:170:VAL:O	1:C:245:PRO:HB3	2.17	0.44
1:E:41:ILE:HG21	1:E:78:ILE:HD11	1.99	0.44
1:A:41:ILE:HG21	1:A:78:ILE:HD11	1.99	0.44
1:A:49:VAL:CG2	1:A:74:ALA:HB2	2.47	0.44
1:A:171:TRP:CE2	1:A:224:HIS:HB2	2.52	0.44
1:C:164:LYS:HE3	5:C:401:NAG:H82	1.99	0.44
2:B:83:TRP:CD2	2:F:66:ILE:HD12	2.52	0.44
1:A:19:LEU:HD21	2:F:102:MET:HE3	1.99	0.44
1:C:281:SER:OG	1:C:283:LEU:HG	2.17	0.44
1:E:171:TRP:CE2	1:E:224:HIS:HB2	2.52	0.44
1:C:211:ARG:HD2	1:C:220:ARG:CG	2.47	0.44
1:E:46:LYS:NZ	1:E:270:GLY:O	2.42	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:ILE:HG21	1:E:170:VAL:HG21	2.00	0.44
1:C:237:SER:HB2	1:E:210:ALA:HB3	2.00	0.43
1:E:49:VAL:CG2	1:E:74:ALA:HB2	2.48	0.43
1:E:33:VAL:HA	1:E:285:PHE:O	2.18	0.43
2:F:168:GLN:O	2:F:171:ILE:N	2.50	0.43
1:A:33:VAL:HA	1:A:285:PHE:O	2.18	0.43
2:B:2:LEU:O	2:B:4:GLY:N	2.48	0.43
2:B:55:LEU:HD22	2:B:99:LEU:HD21	2.00	0.43
2:D:55:LEU:HD22	2:D:99:LEU:HD21	1.99	0.43
2:D:88:ILE:O	2:D:91:VAL:N	2.52	0.43
1:E:282:ASN:HB2	2:F:56:ILE:HG23	1.99	0.43
2:B:102:MET:HE3	1:C:19:LEU:HD21	2.01	0.43
1:E:19:LEU:HD13	2:F:102:MET:CA	2.48	0.43
2:B:142:HIS:CE1	2:B:162:TYR:CG	3.07	0.43
1:C:33:VAL:HA	1:C:285:PHE:O	2.18	0.43
2:D:48:ILE:O	2:D:49:THR:C	2.62	0.43
2:D:66:ILE:HD12	2:F:83:TRP:CD2	2.53	0.43
2:F:88:ILE:O	2:F:91:VAL:N	2.52	0.43
2:F:142:HIS:CE1	2:F:162:TYR:CG	3.07	0.43
1:C:131:ARG:NH1	1:C:136:PHE:O	2.48	0.43
2:F:2:LEU:O	2:F:4:GLY:N	2.48	0.42
1:A:129:CYS:HB2	1:A:135:SER:O	2.19	0.42
2:B:48:ILE:O	2:B:49:THR:C	2.62	0.42
1:C:316:GLU:HG2	2:D:12:ASN:HD21	1.83	0.42
2:D:142:HIS:CE1	2:D:162:TYR:CG	3.07	0.42
1:E:39:PRO:O	1:E:40:ARG:HG3	2.18	0.42
1:C:55:GLY:O	1:C:58:GLY:N	2.52	0.42
2:B:88:ILE:O	2:B:91:VAL:N	2.52	0.42
1:E:129:CYS:HB2	1:E:135:SER:O	2.20	0.42
1:E:219:GLY:O	1:E:220:ARG:NH1	2.52	0.42
1:A:19:LEU:HD13	2:B:102:MET:CA	2.50	0.42
1:C:260:SER:HA	1:C:275:SER:HA	2.01	0.42
2:D:47:GLN:NE2	2:D:110:LEU:HD11	2.35	0.42
2:B:83:TRP:CE2	2:F:66:ILE:CD1	3.03	0.42
1:E:275:SER:OG	2:F:69:GLU:OE2	2.33	0.42
1:A:131:ARG:NH1	1:A:136:PHE:O	2.48	0.41
1:A:260:SER:HA	1:A:275:SER:HA	2.02	0.41
2:D:66:ILE:CD1	2:F:83:TRP:CE2	3.03	0.41
2:D:127:ARG:HG3	2:D:159:HIS:CD2	2.55	0.41
1:C:129:CYS:HB2	1:C:135:SER:O	2.19	0.41
2:F:47:GLN:NE2	2:F:110:LEU:HD11	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:MET:HA	1:A:256:MET:CE	2.46	0.41
2:B:66:ILE:CD1	2:D:83:TRP:CE2	3.04	0.41
2:F:127:ARG:HG3	2:F:159:HIS:CD2	2.56	0.41
1:C:219:GLY:O	1:C:220:ARG:NH1	2.53	0.41
2:B:168:GLN:O	2:B:171:ILE:N	2.51	0.41
2:D:168:GLN:O	2:D:169:ASN:C	2.63	0.41
1:E:44:LYS:HE2	1:E:269:GLU:HB2	2.03	0.41
1:E:260:SER:HA	1:E:275:SER:HA	2.02	0.41
2:F:48:ILE:O	2:F:49:THR:C	2.62	0.41
2:F:168:GLN:O	2:F:169:ASN:C	2.63	0.41
2:B:168:GLN:O	2:B:169:ASN:C	2.63	0.40
1:A:287:ASN:O	1:A:287:ASN:CG	2.64	0.40
2:B:127:ARG:HG3	2:B:159:HIS:CD2	2.56	0.40
1:E:192:LEU:HD12	1:E:205:VAL:CG2	2.51	0.40
1:A:90:GLY:HA3	1:A:221:ILE:O	2.21	0.40
1:C:170:VAL:HG12	1:C:171:TRP:N	2.37	0.40
1:E:55:GLY:O	1:E:58:GLY:N	2.53	0.40
1:E:182:GLN:OE1	1:E:206:PRO:HG2	2.21	0.40
1:C:93:VAL:HG11	1:C:224:HIS:CD2	2.57	0.40
2:D:77:ILE:HD11	2:F:80:VAL:HG21	2.04	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	314/321 (98%)	268 (85%)	35 (11%)	11 (4%)	3	23
1	C	314/321 (98%)	268 (85%)	36 (12%)	10 (3%)	3	24
1	E	314/321 (98%)	268 (85%)	36 (12%)	10 (3%)	3	24
2	B	169/221 (76%)	140 (83%)	20 (12%)	9 (5%)	1	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	169/221 (76%)	140 (83%)	20 (12%)	9 (5%)	1	14
2	F	169/221 (76%)	140 (83%)	21 (12%)	8 (5%)	2	17
All	All	1449/1626 (89%)	1224 (84%)	168 (12%)	57 (4%)	2	20

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	29	ALA
2	B	127	ARG
2	B	142	HIS
2	D	29	ALA
2	D	127	ARG
2	D	142	HIS
2	F	29	ALA
2	F	127	ARG
2	F	142	HIS
1	A	27	VAL
1	A	42	CYS
1	A	184	LYS
1	A	190	ASN
1	A	202	GLN
1	A	241	ALA
2	B	89	THR
1	C	27	VAL
1	C	42	CYS
1	C	184	LYS
1	C	190	ASN
1	C	202	GLN
1	C	241	ALA
2	D	89	THR
1	E	27	VAL
1	E	42	CYS
1	E	184	LYS
1	E	190	ASN
1	E	202	GLN
1	E	241	ALA
2	F	89	THR
1	A	161	ASN
2	B	7	ALA
2	B	157	TYR
1	C	161	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	7	ALA
2	D	157	TYR
1	E	161	ASN
1	E	200	TYR
2	F	7	ALA
2	F	157	TYR
1	A	200	TYR
2	B	170	ARG
1	C	200	TYR
2	D	3	PHE
2	D	170	ARG
2	B	3	PHE
2	F	3	PHE
2	F	170	ARG
2	B	2	LEU
2	D	2	LEU
1	E	177	VAL
1	A	177	VAL
1	C	177	VAL
1	C	64	PRO
1	A	64	PRO
1	A	315	PRO
1	E	64	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	267/271 (98%)	222 (83%)	45 (17%)	2	13
1	C	267/271 (98%)	224 (84%)	43 (16%)	2	14
1	E	267/271 (98%)	222 (83%)	45 (17%)	2	13
2	B	145/189 (77%)	129 (89%)	16 (11%)	6	27
2	D	145/189 (77%)	131 (90%)	14 (10%)	8	31
2	F	145/189 (77%)	132 (91%)	13 (9%)	9	33

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1236/1380 (90%)	1060 (86%)	176 (14%)	3 19

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	10	VAL
1	A	12	ASN
1	A	14	THR
1	A	18	THR
1	A	19	LEU
1	A	21	GLU
1	A	24	VAL
1	A	32	THR
1	A	36	THR
1	A	53	GLN
1	A	65	GLN
1	A	81	ARG
1	A	85	ASP
1	A	86	VAL
1	A	93	VAL
1	A	108	ILE
1	A	112	THR
1	A	116	THR
1	A	122	THR
1	A	125	VAL
1	A	130	LYS
1	A	141	LYS
1	A	146	ASN
1	A	176	SER
1	A	177	VAL
1	A	194	THR
1	A	199	ASN
1	A	200	TYR
1	A	202	GLN
1	A	217	LEU
1	A	231	ASN
1	A	237	SER
1	A	249	SER
1	A	256	MET
1	A	262	VAL
1	A	263	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	265	ASP
1	A	268	CYS
1	A	275	SER
1	A	282	ASN
1	A	291	ARG
1	A	298	ARG
1	A	312	LYS
1	A	314	VAL
2	B	19	ASP
2	B	39	LYS
2	B	52	LEU
2	B	59	THR
2	B	60	ASN
2	B	66	ILE
2	B	69	GLU
2	B	75	LYS
2	B	87	SER
2	B	115	MET
2	B	117	LYS
2	B	129	ASN
2	B	133	ASP
2	B	140	ILE
2	B	147	ASP
2	B	169	ASN
1	C	8	HIS
1	C	10	VAL
1	C	12	ASN
1	C	14	THR
1	C	18	THR
1	C	19	LEU
1	C	21	GLU
1	C	24	VAL
1	C	32	THR
1	C	36	THR
1	C	53	GLN
1	C	65	GLN
1	C	81	ARG
1	C	85	ASP
1	C	86	VAL
1	C	93	VAL
1	C	108	ILE
1	C	112	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	116	THR
1	C	122	THR
1	C	125	VAL
1	C	130	LYS
1	C	141	LYS
1	C	146	ASN
1	C	176	SER
1	C	177	VAL
1	C	194	THR
1	C	199	ASN
1	C	200	TYR
1	C	202	GLN
1	C	217	LEU
1	C	231	ASN
1	C	237	SER
1	C	249	SER
1	C	256	MET
1	C	262	VAL
1	C	263	GLN
1	C	268	CYS
1	C	275	SER
1	C	282	ASN
1	C	291	ARG
1	C	312	LYS
1	C	314	VAL
2	D	19	ASP
2	D	39	LYS
2	D	52	LEU
2	D	60	ASN
2	D	66	ILE
2	D	72	GLU
2	D	87	SER
2	D	90	GLU
2	D	115	MET
2	D	117	LYS
2	D	129	ASN
2	D	133	ASP
2	D	140	ILE
2	D	147	ASP
1	E	8	HIS
1	E	10	VAL
1	E	12	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	14	THR
1	E	18	THR
1	E	19	LEU
1	E	24	VAL
1	E	32	THR
1	E	36	THR
1	E	53	GLN
1	E	65	GLN
1	E	81	ARG
1	E	85	ASP
1	E	86	VAL
1	E	93	VAL
1	E	108	ILE
1	E	112	THR
1	E	116	THR
1	E	122	THR
1	E	125	VAL
1	E	130	LYS
1	E	141	LYS
1	E	146	ASN
1	E	176	SER
1	E	177	VAL
1	E	182	GLN
1	E	194	THR
1	E	199	ASN
1	E	200	TYR
1	E	202	GLN
1	E	217	LEU
1	E	231	ASN
1	E	237	SER
1	E	249	SER
1	E	256	MET
1	E	262	VAL
1	E	263	GLN
1	E	268	CYS
1	E	275	SER
1	E	282	ASN
1	E	291	ARG
1	E	298	ARG
1	E	307	LEU
1	E	312	LYS
1	E	314	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	19	ASP
2	F	39	LYS
2	F	52	LEU
2	F	58	LYS
2	F	60	ASN
2	F	66	ILE
2	F	87	SER
2	F	115	MET
2	F	117	LYS
2	F	129	ASN
2	F	133	ASP
2	F	140	ILE
2	F	147	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	146	ASN
1	A	175	HIS
1	A	263	GLN
2	B	28	ASN
2	B	60	ASN
2	B	62	GLN
2	B	105	GLN
2	B	159	HIS
1	C	8	HIS
1	C	17	ASN
1	C	94	ASN
1	C	146	ASN
1	C	175	HIS
1	C	263	GLN
2	D	28	ASN
2	D	154	ASN
2	D	159	HIS
1	E	8	HIS
1	E	94	ASN
1	E	146	ASN
1	E	175	HIS
2	F	28	ASN
2	F	105	GLN
2	F	154	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	159	HIS

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 ⓘ

8 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	14,14,15	1.30	2 (14%)	17,19,21	2.58	6 (35%)
3	GAL	G	2	3	11,11,12	0.74	0	15,15,17	1.32	3 (20%)
3	SIA	G	3	3	20,20,21	1.38	3 (15%)	21,28,31	1.94	8 (38%)
3	NAG	H	1	3	14,14,15	1.31	2 (14%)	17,19,21	2.58	6 (35%)
3	GAL	H	2	3	11,11,12	0.73	0	15,15,17	1.32	3 (20%)
3	SIA	H	3	3	20,20,21	1.37	3 (15%)	21,28,31	1.95	8 (38%)
4	NAG	I	1	4	14,14,15	1.28	2 (14%)	17,19,21	2.65	5 (29%)
4	GAL	I	2	4	11,11,12	0.61	0	15,15,17	1.27	2 (13%)

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	-	2/6/23/26	0/1/1/1
3	GAL	G	2	3	-	2/2/19/22	0/1/1/1
3	SIA	G	3	3	-	3/18/34/38	0/1/1/1
3	NAG	H	1	3	-	2/6/23/26	0/1/1/1
3	GAL	H	2	3	-	2/2/19/22	0/1/1/1
3	SIA	H	3	3	-	3/18/34/38	0/1/1/1
4	NAG	I	1	4	-	1/6/23/26	0/1/1/1
4	GAL	I	2	4	-	1/2/19/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	3	SIA	C7-C6	3.52	1.57	1.52
3	H	3	SIA	C7-C6	3.46	1.57	1.52
4	I	1	NAG	O6-C6	2.73	1.53	1.42
3	H	1	NAG	C3-C2	2.23	1.57	1.52
3	H	3	SIA	C8-C7	2.21	1.57	1.53
3	G	3	SIA	C8-C7	2.21	1.57	1.53
3	G	1	NAG	C3-C2	2.20	1.57	1.52
4	I	1	NAG	C2-N2	2.17	1.49	1.46
3	G	1	NAG	C2-N2	2.05	1.49	1.46
3	H	1	NAG	C2-N2	2.04	1.49	1.46
3	G	3	SIA	O6-C6	2.02	1.47	1.44
3	H	3	SIA	O6-C6	2.02	1.47	1.44

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1	NAG	O3-C3-C4	7.49	128.02	110.38
3	H	1	NAG	O3-C3-C2	7.46	124.89	109.40
3	G	1	NAG	O3-C3-C2	7.45	124.88	109.40
4	I	1	NAG	C4-C3-C2	4.32	117.35	111.02
3	H	3	SIA	C6-C5-N5	3.95	117.20	110.91
3	G	3	SIA	C6-C5-N5	3.94	117.19	110.91
4	I	2	GAL	C1-O5-C5	3.77	117.24	112.19
4	I	1	NAG	C2-N2-C7	3.72	127.88	122.90
3	G	1	NAG	O3-C3-C4	3.71	119.12	110.38
3	H	1	NAG	O3-C3-C4	3.70	119.10	110.38
3	H	3	SIA	O6-C2-C1	3.55	114.43	107.72
3	G	3	SIA	O6-C2-C1	3.53	114.39	107.72
3	H	3	SIA	C11-C10-N5	3.14	121.33	116.12
3	G	3	SIA	C11-C10-N5	3.11	121.28	116.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1	NAG	C2-N2-C7	3.08	127.03	122.90
3	H	1	NAG	C2-N2-C7	3.07	127.02	122.90
3	G	2	GAL	C1-O5-C5	2.90	116.07	112.19
3	H	2	GAL	C1-O5-C5	2.90	116.07	112.19
3	H	3	SIA	C8-C7-C6	2.89	118.49	113.05
3	G	3	SIA	C8-C7-C6	2.88	118.47	113.05
4	I	2	GAL	C1-C2-C3	2.59	113.42	109.64
4	I	1	NAG	O5-C5-C6	2.57	112.67	107.66
4	I	1	NAG	C3-C4-C5	2.56	114.88	110.23
3	G	3	SIA	O1B-C1-C2	2.55	119.34	112.71
3	H	3	SIA	O1B-C1-C2	2.54	119.32	112.71
3	G	1	NAG	C3-C4-C5	2.49	114.75	110.23
3	H	1	NAG	C3-C4-C5	2.48	114.72	110.23
3	G	1	NAG	O6-C6-C5	2.41	119.55	111.33
3	H	1	NAG	O6-C6-C5	2.41	119.54	111.33
3	H	2	GAL	O5-C5-C6	2.38	112.29	107.66
3	G	2	GAL	O5-C5-C6	2.38	112.29	107.66
3	G	3	SIA	O1A-C1-C2	-2.28	117.92	122.85
3	H	3	SIA	O1A-C1-C2	-2.27	117.95	122.85
3	H	3	SIA	C4-C5-N5	-2.21	106.08	110.44
3	G	3	SIA	C4-C5-N5	-2.20	106.10	110.44
3	H	2	GAL	C1-C2-C3	2.14	112.77	109.64
3	G	2	GAL	C1-C2-C3	2.13	112.75	109.64
3	H	1	NAG	C4-C3-C2	2.03	114.00	111.02
3	G	1	NAG	C4-C3-C2	2.03	113.99	111.02
3	G	3	SIA	C5-N5-C10	2.02	127.84	123.11
3	H	3	SIA	C5-N5-C10	2.01	127.81	123.11

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	1	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	G	2	GAL	O5-C5-C6-O6
3	H	2	GAL	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	G	2	GAL	C4-C5-C6-O6
3	H	2	GAL	C4-C5-C6-O6
3	G	3	SIA	C11-C10-N5-C5
3	G	3	SIA	O10-C10-N5-C5

Continued on next page...

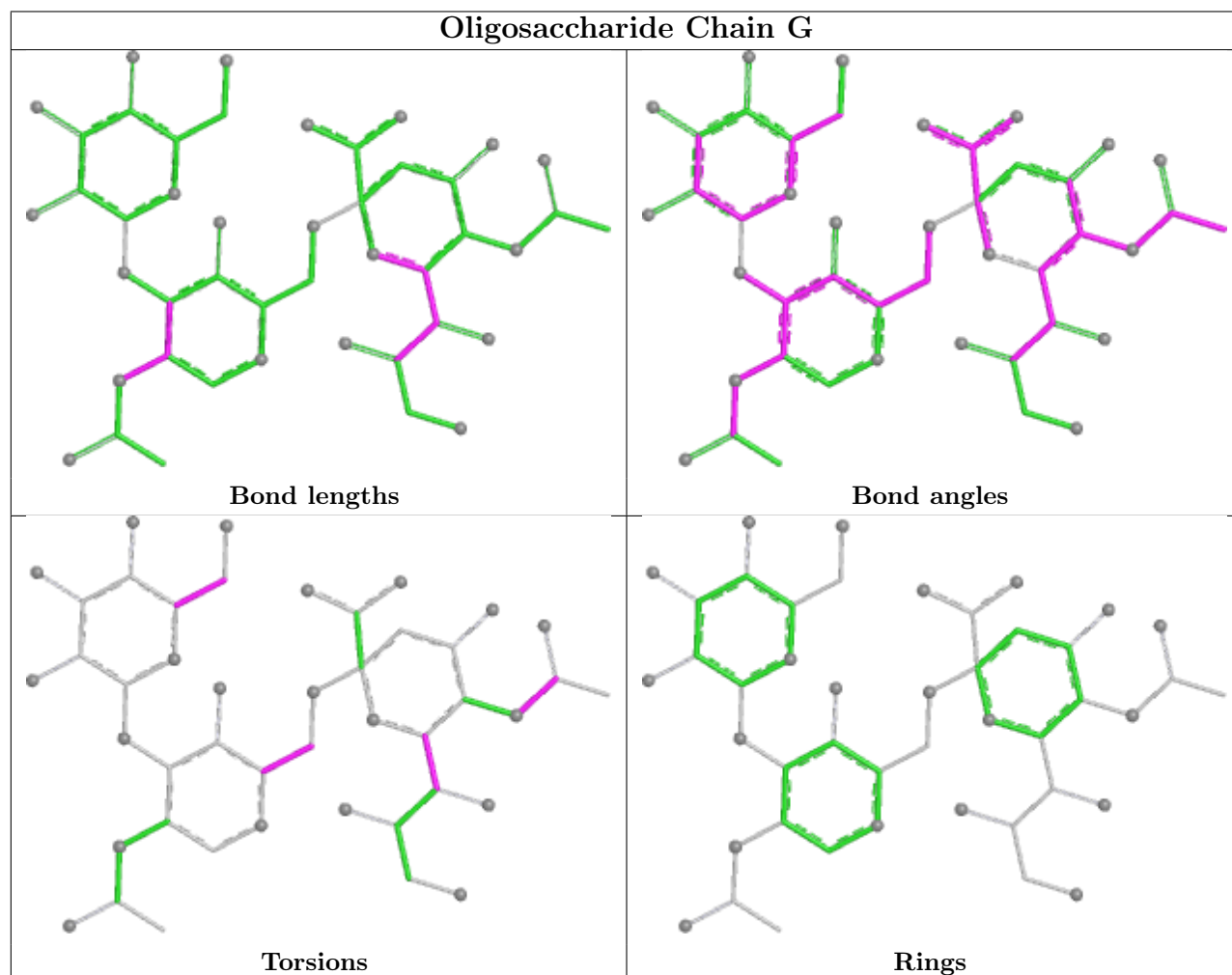
Continued from previous page...

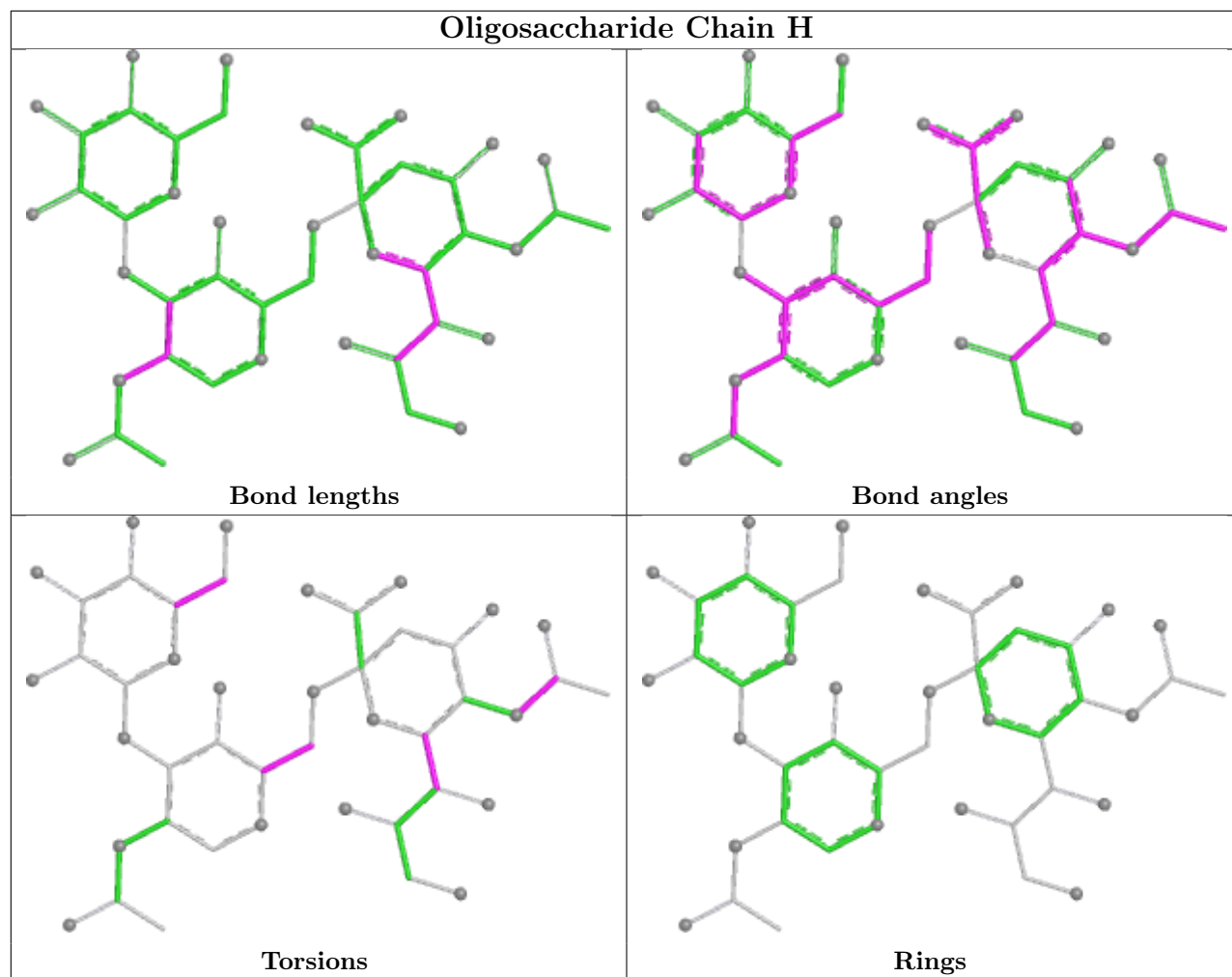
Mol	Chain	Res	Type	Atoms
3	H	3	SIA	C11-C10-N5-C5
3	H	3	SIA	O10-C10-N5-C5
4	I	1	NAG	O5-C5-C6-O6
4	I	2	GAL	O5-C5-C6-O6
3	G	3	SIA	O6-C6-C7-O7
3	H	3	SIA	O6-C6-C7-O7

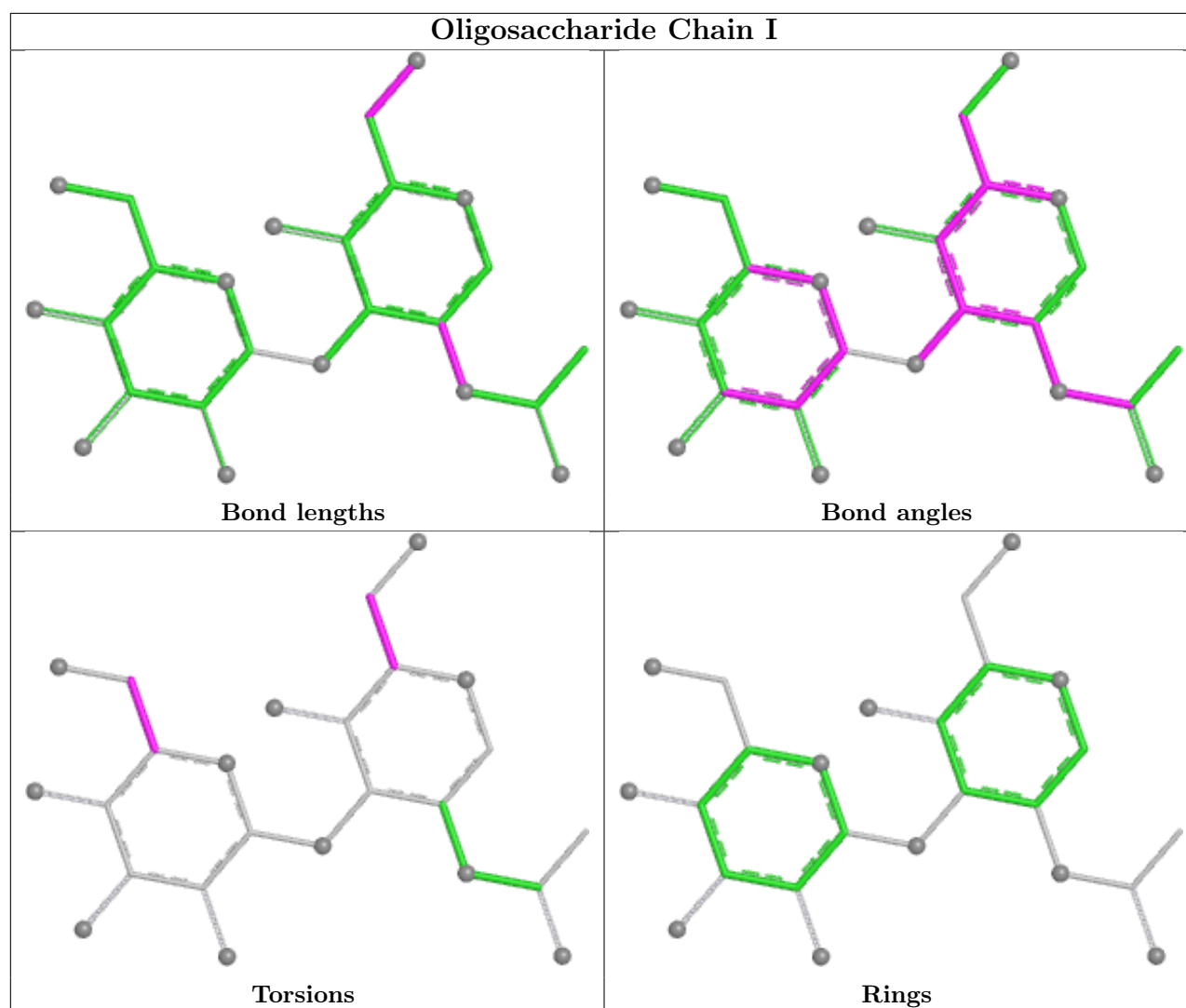
There are no ring outliers.

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.







5.6 Ligand geometry [i](#)

10 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	F	301	2	14,14,15	1.80	3 (21%)	17,19,21	3.83	10 (58%)
5	NAG	B	301	2	14,14,15	1.27	1 (7%)	17,19,21	2.69	6 (35%)
6	GAL	E	405	-	12,12,12	0.73	0	17,17,17	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	401	1	14,14,15	1.10	1 (7%)	17,19,21	2.09	6 (35%)
5	NAG	E	401	1	14,14,15	1.06	1 (7%)	17,19,21	1.73	1 (5%)
5	NAG	A	401	1	14,14,15	1.25	1 (7%)	17,19,21	2.29	5 (29%)
6	GAL	A	405	-	12,12,12	0.82	0	17,17,17	1.17	1 (5%)
5	NAG	D	301	2	14,14,15	1.64	2 (14%)	17,19,21	3.02	9 (52%)
7	SIA	E	402	-	20,20,21	1.58	3 (15%)	21,28,31	2.13	7 (33%)
6	GAL	C	405	-	12,12,12	0.82	0	17,17,17	1.17	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	F	301	2	-	2/6/23/26	0/1/1/1
5	NAG	B	301	2	-	2/6/23/26	0/1/1/1
6	GAL	E	405	-	-	0/2/22/22	0/1/1/1
5	NAG	C	401	1	-	3/6/23/26	0/1/1/1
5	NAG	E	401	1	-	3/6/23/26	0/1/1/1
5	NAG	A	401	1	-	4/6/23/26	0/1/1/1
6	GAL	A	405	-	-	2/2/22/22	0/1/1/1
5	NAG	D	301	2	-	0/6/23/26	0/1/1/1
7	SIA	E	402	-	-	3/18/34/38	0/1/1/1
6	GAL	C	405	-	-	2/2/22/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	402	SIA	C7-C6	4.43	1.58	1.52
5	F	301	NAG	O5-C1	3.80	1.50	1.43
7	E	402	SIA	O6-C6	3.13	1.48	1.44
5	F	301	NAG	C1-C2	3.10	1.56	1.52
5	D	301	NAG	C1-C2	3.08	1.56	1.52
5	A	401	NAG	C2-N2	2.67	1.50	1.46
5	F	301	NAG	O5-C5	2.63	1.48	1.43
5	D	301	NAG	O5-C1	2.59	1.48	1.43
7	E	402	SIA	C6-C5	2.59	1.57	1.53
5	B	301	NAG	O5-C1	2.37	1.47	1.43
5	C	401	NAG	C1-C2	2.22	1.55	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	401	NAG	C2-N2	2.15	1.49	1.46

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	301	NAG	C1-C2-N2	10.55	127.05	110.43
5	B	301	NAG	C1-O5-C5	8.61	123.72	112.19
5	D	301	NAG	C1-C2-N2	8.06	123.14	110.43
5	F	301	NAG	C1-O5-C5	6.93	121.47	112.19
5	A	401	NAG	C2-N2-C7	6.84	132.06	122.90
5	E	401	NAG	C2-N2-C7	5.63	130.45	122.90
5	F	301	NAG	O5-C5-C6	5.18	117.75	107.66
5	D	301	NAG	C1-O5-C5	4.56	118.30	112.19
7	E	402	SIA	C8-C7-C6	4.41	121.34	113.05
5	C	401	NAG	C2-N2-C7	4.22	128.55	122.90
5	D	301	NAG	C3-C4-C5	-4.00	102.97	110.23
7	E	402	SIA	O6-C2-C1	3.97	115.21	107.72
5	A	401	NAG	C1-C2-N2	3.93	116.63	110.43
5	C	401	NAG	C4-C3-C2	3.82	116.61	111.02
5	C	401	NAG	O5-C1-C2	3.71	117.04	111.29
5	F	301	NAG	O5-C1-C2	-3.52	105.85	111.29
5	F	301	NAG	C4-C3-C2	-3.51	105.87	111.02
7	E	402	SIA	C11-C10-N5	3.49	121.91	116.12
5	D	301	NAG	O5-C5-C6	3.49	114.45	107.66
5	B	301	NAG	C1-C2-N2	3.13	115.36	110.43
5	B	301	NAG	C4-C3-C2	-2.93	106.73	111.02
7	E	402	SIA	O1A-C1-C2	-2.91	116.57	122.85
7	E	402	SIA	O1B-C1-C2	2.84	120.09	112.71
5	F	301	NAG	C3-C4-C5	-2.83	105.09	110.23
5	C	401	NAG	O7-C7-N2	2.81	126.94	121.98
5	D	301	NAG	O4-C4-C5	2.79	116.20	109.32
7	E	402	SIA	O6-C2-C3	2.69	114.17	110.56
5	C	401	NAG	O7-C7-C8	-2.67	117.29	122.05
5	F	301	NAG	O4-C4-C3	2.65	116.61	110.38
5	A	401	NAG	C1-O5-C5	2.61	115.69	112.19
5	D	301	NAG	O7-C7-C8	-2.55	117.52	122.05
5	A	401	NAG	O7-C7-C8	-2.54	117.52	122.05
7	E	402	SIA	C5-N5-C10	2.53	129.03	123.11
5	D	301	NAG	O4-C4-C3	2.53	116.33	110.38
5	B	301	NAG	O4-C4-C5	2.51	115.51	109.32
6	A	405	GAL	C3-C4-C5	2.49	114.75	110.23
6	C	405	GAL	C3-C4-C5	2.48	114.73	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	401	NAG	O7-C7-N2	2.40	126.23	121.98
5	F	301	NAG	O3-C3-C4	2.34	115.90	110.38
5	D	301	NAG	C4-C3-C2	-2.28	107.68	111.02
5	D	301	NAG	O7-C7-N2	2.26	125.97	121.98
5	F	301	NAG	C6-C5-C4	-2.18	107.67	113.02
5	F	301	NAG	O7-C7-N2	2.11	125.71	121.98
5	B	301	NAG	O5-C5-C4	2.10	115.95	110.83
5	B	301	NAG	O7-C7-C8	-2.09	118.34	122.05
5	C	401	NAG	C1-O5-C5	2.05	114.93	112.19

There are no chirality outliers.

All (21) torsion outliers are listed below:

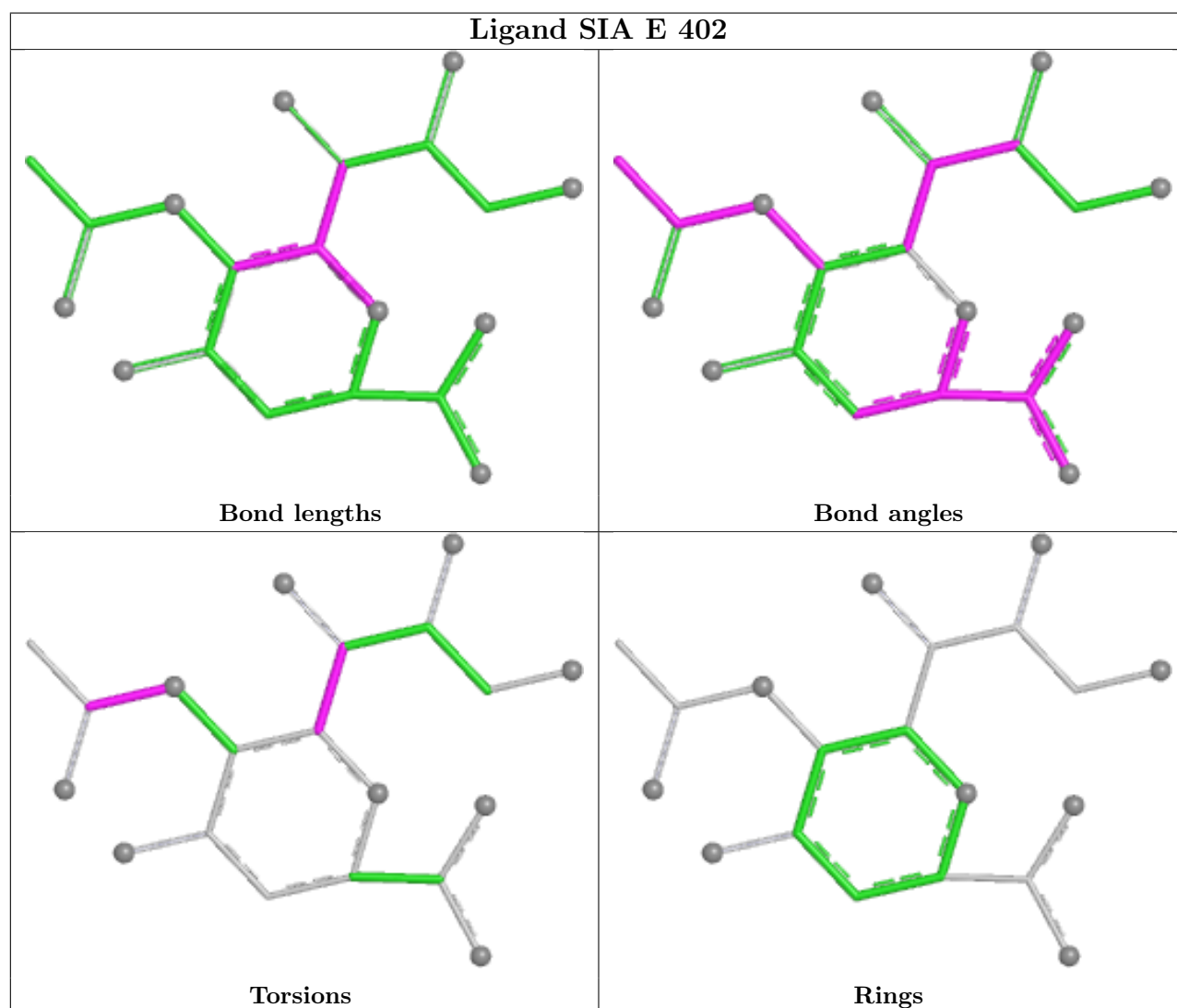
Mol	Chain	Res	Type	Atoms
5	C	401	NAG	C1-C2-N2-C7
7	E	402	SIA	O6-C6-C7-O7
5	F	301	NAG	O5-C5-C6-O6
5	F	301	NAG	C4-C5-C6-O6
5	A	401	NAG	O5-C5-C6-O6
5	E	401	NAG	O5-C5-C6-O6
6	A	405	GAL	O5-C5-C6-O6
6	C	405	GAL	O5-C5-C6-O6
5	B	301	NAG	O5-C5-C6-O6
6	A	405	GAL	C4-C5-C6-O6
6	C	405	GAL	C4-C5-C6-O6
5	E	401	NAG	C4-C5-C6-O6
7	E	402	SIA	C11-C10-N5-C5
7	E	402	SIA	O10-C10-N5-C5
5	A	401	NAG	C4-C5-C6-O6
5	B	301	NAG	C4-C5-C6-O6
5	C	401	NAG	O5-C5-C6-O6
5	C	401	NAG	C3-C2-N2-C7
5	E	401	NAG	C3-C2-N2-C7
5	A	401	NAG	C3-C2-N2-C7
5	A	401	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	401	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 [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	316/321 (98%)	0.01	1 (0%)	90 74	19, 59, 116, 145	1 (0%)
1	C	316/321 (98%)	-0.02	3 (0%)	81 56	18, 60, 112, 145	1 (0%)
1	E	316/321 (98%)	0.02	3 (0%)	81 56	20, 59, 116, 148	1 (0%)
2	B	171/221 (77%)	0.29	1 (0%)	85 63	17, 94, 134, 150	0
2	D	171/221 (77%)	0.28	2 (1%)	76 49	20, 90, 135, 153	0
2	F	171/221 (77%)	0.29	2 (1%)	76 49	22, 95, 134, 157	0
All	All	1461/1626 (89%)	0.10	12 (0%)	82 58	17, 71, 128, 157	3 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	149	ASN	3.2
1	A	149	ASN	2.9
1	C	149	ASN	2.7
2	D	138	PHE	2.6
2	B	35	ALA	2.2
2	F	171	ILE	2.2
1	E	201	GLN	2.2
2	F	23	GLY	2.1
1	C	224	HIS	2.1
2	D	141	PHE	2.1
1	E	222	ASP	2.0
1	C	201	GLN	2.0

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

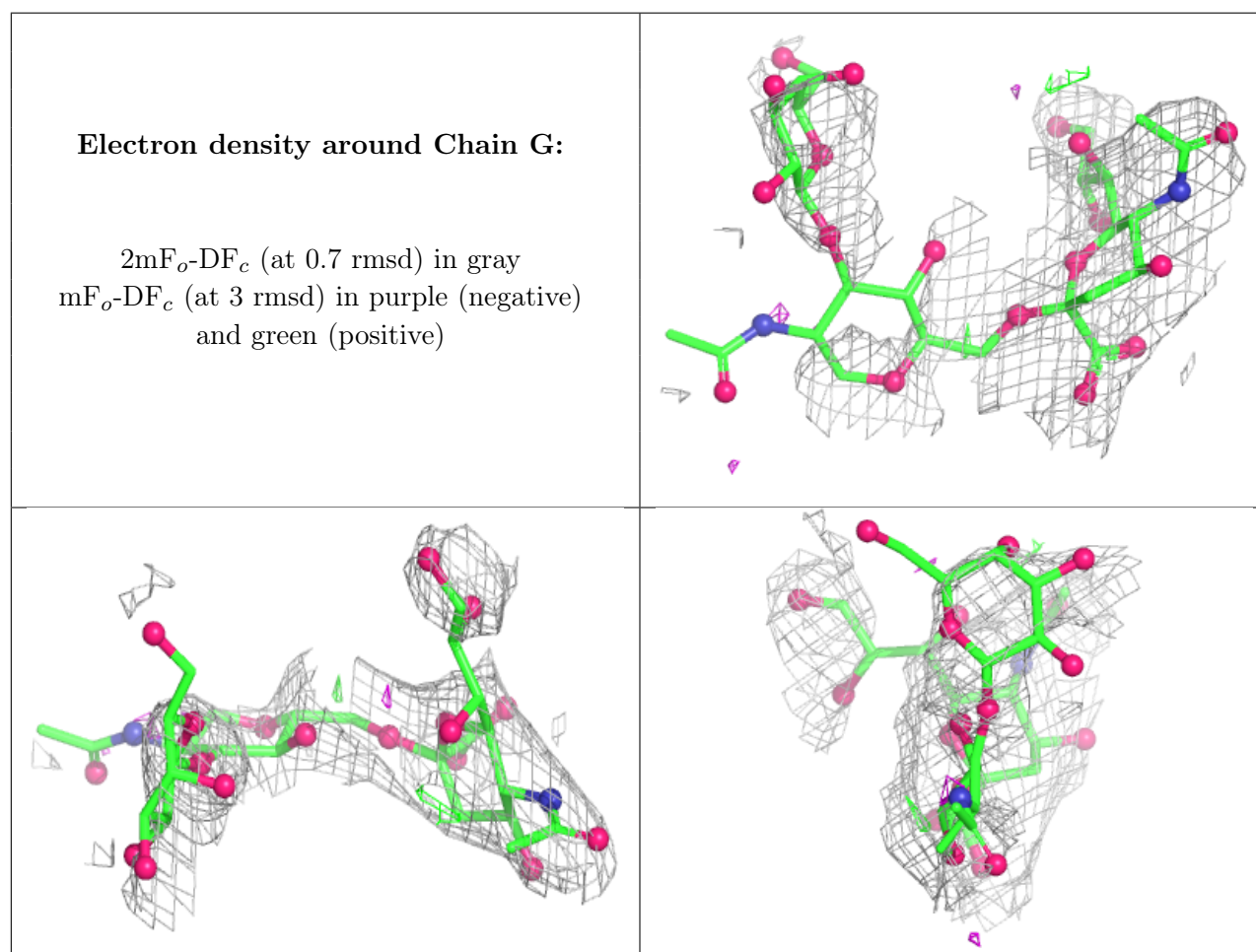
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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.

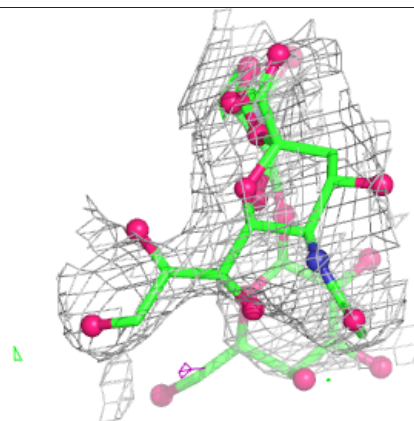
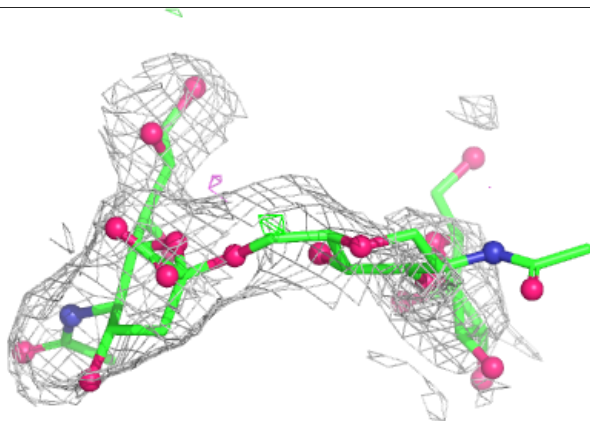
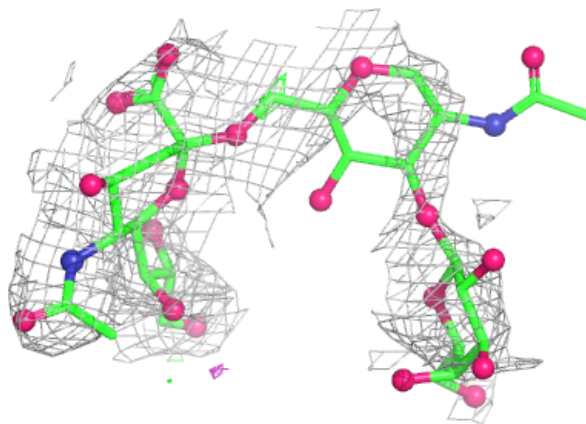
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	H	1	14/15	0.49	0.19	129,144,153,156	0
4	NAG	I	1	14/15	0.51	0.18	130,142,151,161	0
3	NAG	G	1	14/15	0.53	0.18	129,144,153,156	0
3	GAL	H	2	11/12	0.67	0.15	143,153,154,154	0
4	GAL	I	2	11/12	0.67	0.14	153,161,163,165	0
3	GAL	G	2	11/12	0.68	0.15	143,153,154,154	0
3	SIA	G	3	20/21	0.77	0.14	93,117,127,128	0
3	SIA	H	3	20/21	0.77	0.15	93,117,127,128	0

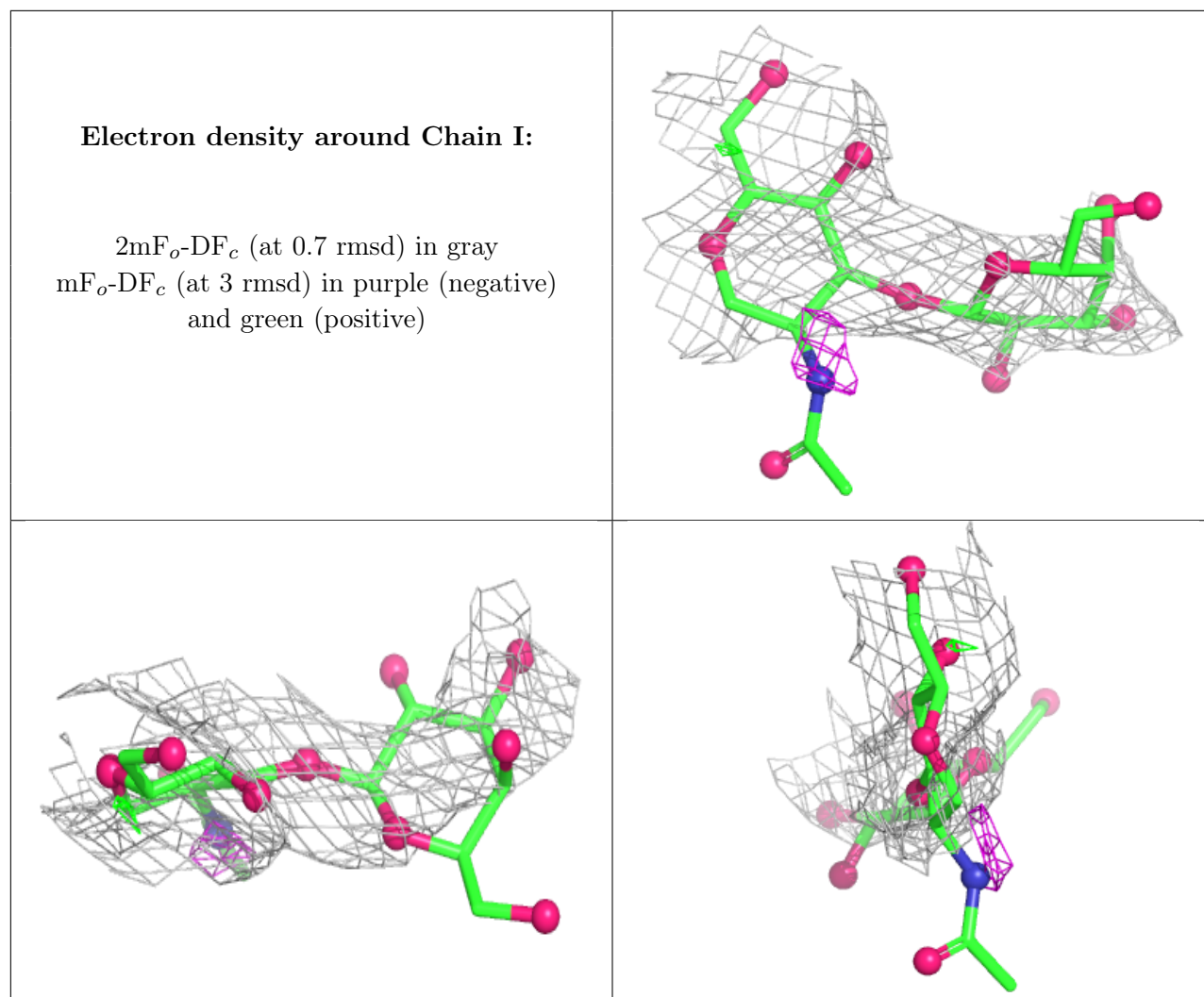
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain H:

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





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.

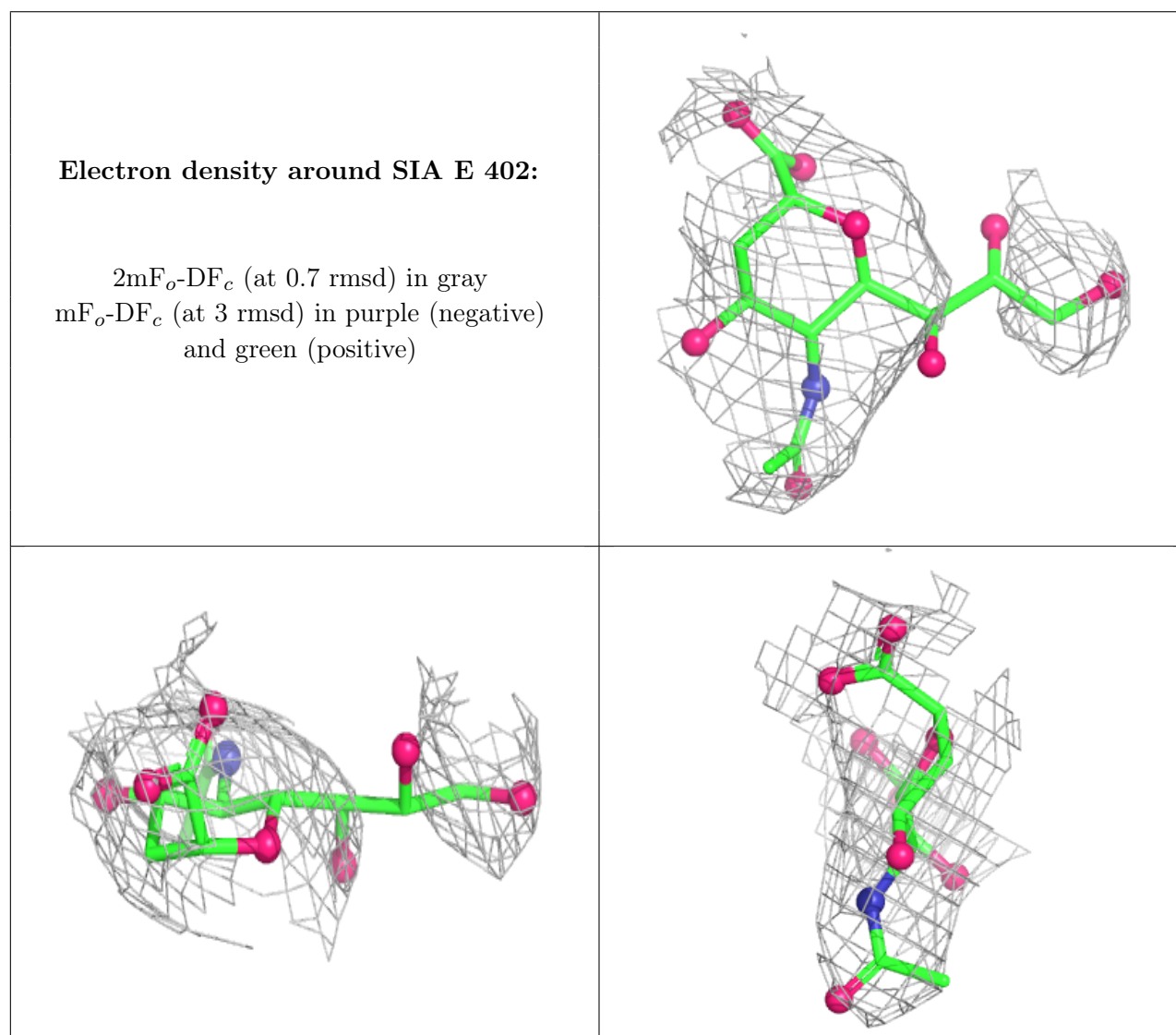
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GAL	C	405	12/12	0.42	0.16	122,133,139,140	0
6	GAL	A	405	12/12	0.55	0.13	122,133,139,140	0
6	GAL	E	405	12/12	0.57	0.13	121,137,142,142	0
5	NAG	A	401	14/15	0.60	0.14	111,124,135,144	0
5	NAG	C	401	14/15	0.66	0.12	115,124,137,137	0
5	NAG	E	401	14/15	0.75	0.11	113,132,143,150	0
7	SIA	E	402	20/21	0.84	0.14	101,121,126,129	0
5	NAG	D	301	14/15	0.87	0.11	50,55,61,65	0
5	NAG	F	301	14/15	0.87	0.11	54,60,63,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	B	301	14/15	0.88	0.11	54,62,69,73	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.