



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 29, 2024 – 11:49 AM EDT

PDB ID : 4KDO
Title : Crystal structure of the hemagglutinin of ferret-transmissible H5N1 virus in complex with human receptor analog LSTc
Authors : Lu, X.; Shi, Y.; Zhang, W.; Zhang, Y.; Qi, J.; Gao, G.F.
Deposited on : 2013-04-25
Resolution : 2.40 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

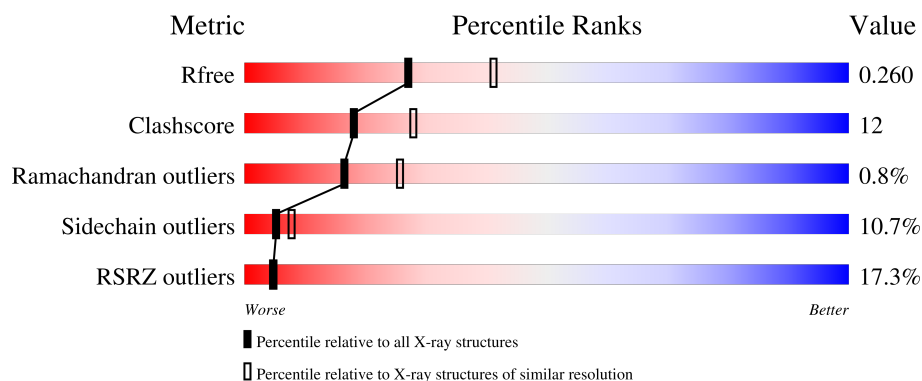
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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.




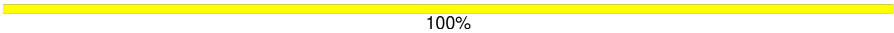

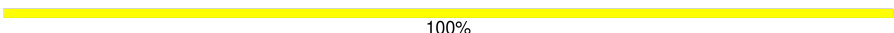

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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	322	<div> <div>11%</div> <div> <div></div> <div>69%</div> <div>25%</div> <div>6%</div> </div> </div>
1	C	322	<div> <div>11%</div> <div> <div></div> <div>70%</div> <div>24%</div> <div>7%</div> </div> </div>
1	E	322	<div> <div>12%</div> <div> <div></div> <div>70%</div> <div>23%</div> <div>7%</div> </div> </div>
2	B	175	<div> <div>36%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>5%</div> </div> </div>
2	D	175	<div> <div>34%</div> <div> <div></div> <div>73%</div> <div>25%</div> <div>.</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	175	
3	G	2	
3	H	2	
3	J	2	
4	I	3	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12373 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	322	Total	C	N	O	S	0	0	0
			2559	1621	440	483	15			
1	C	322	Total	C	N	O	S	0	0	0
			2559	1621	440	483	15			
1	E	322	Total	C	N	O	S	0	0	0
			2559	1621	440	483	15			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLN	-	expression tag	UNP Q6DQ33
A	158	ASP	ASN	engineered mutation	UNP Q6DQ33
A	224	LYS	ASN	engineered mutation	UNP Q6DQ33
A	226	LEU	GLN	engineered mutation	UNP Q6DQ33
A	319	ILE	THR	engineered mutation	UNP Q6DQ33
C	4	GLN	-	expression tag	UNP Q6DQ33
C	158	ASP	ASN	engineered mutation	UNP Q6DQ33
C	224	LYS	ASN	engineered mutation	UNP Q6DQ33
C	226	LEU	GLN	engineered mutation	UNP Q6DQ33
C	319	ILE	THR	engineered mutation	UNP Q6DQ33
E	4	GLN	-	expression tag	UNP Q6DQ33
E	158	ASP	ASN	engineered mutation	UNP Q6DQ33
E	224	LYS	ASN	engineered mutation	UNP Q6DQ33
E	226	LEU	GLN	engineered mutation	UNP Q6DQ33
E	319	ILE	THR	engineered mutation	UNP Q6DQ33

- Molecule 2 is a protein called Hemagglutinin.

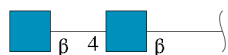
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			

Continued on next page...

Continued from previous page...

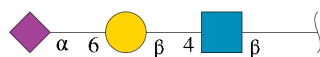
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	F	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			

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



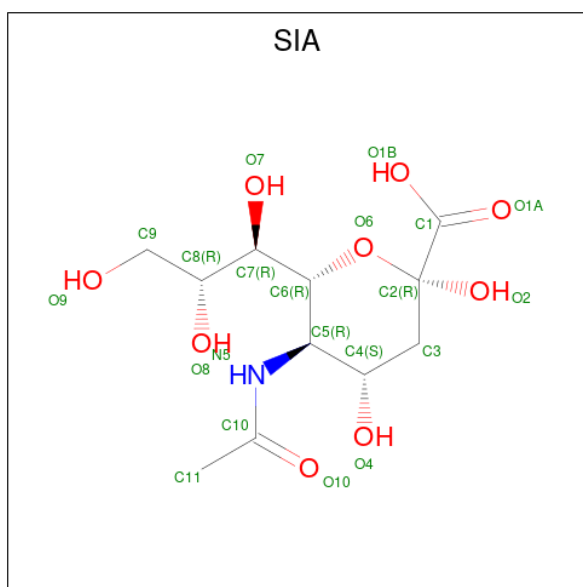
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



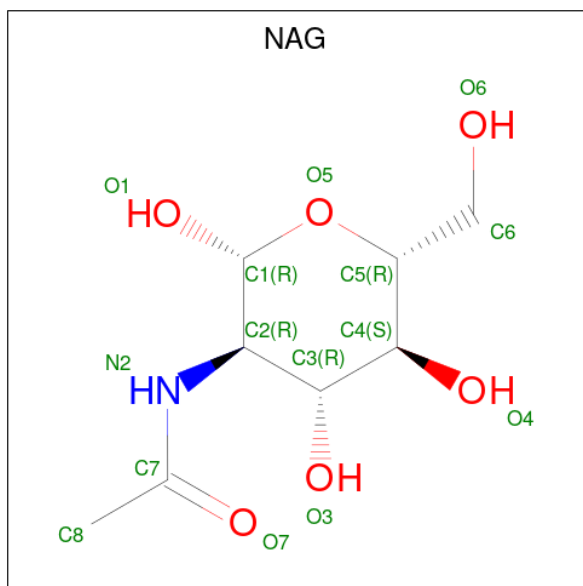
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	3	Total	C	N	O	0	0	0
			46	25	2	19			

- Molecule 5 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: C₁₁H₁₉NO₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

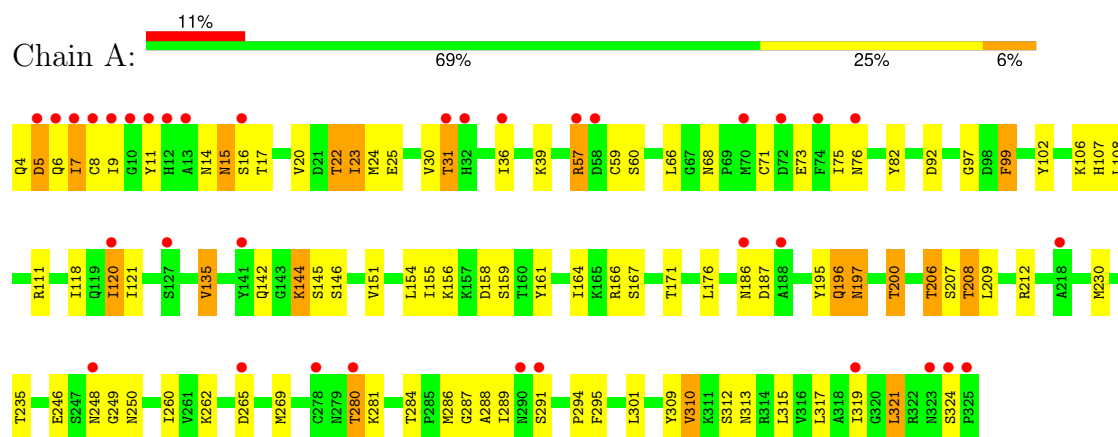
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	80	Total 80	O 80	0	0
7	C	80	Total 80	O 80	0	0
7	E	64	Total 64	O 64	0	0
7	B	24	Total 24	O 24	0	0
7	D	22	Total 22	O 22	0	0
7	F	13	Total 13	O 13	0	0

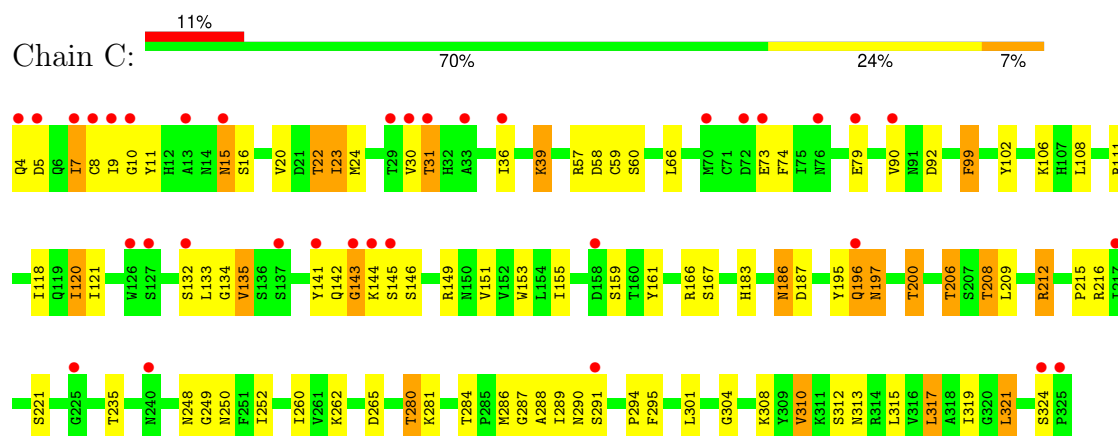
3 Residue-property plots [i](#)

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.

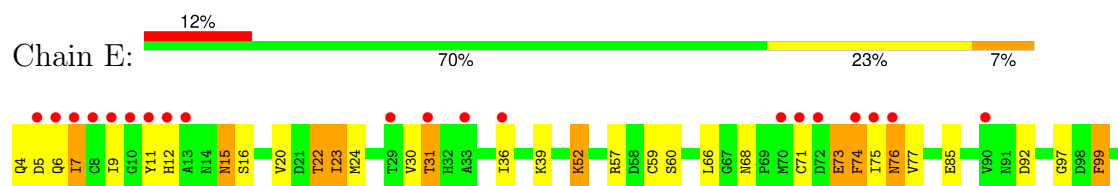
• Molecule 1: Hemagglutinin

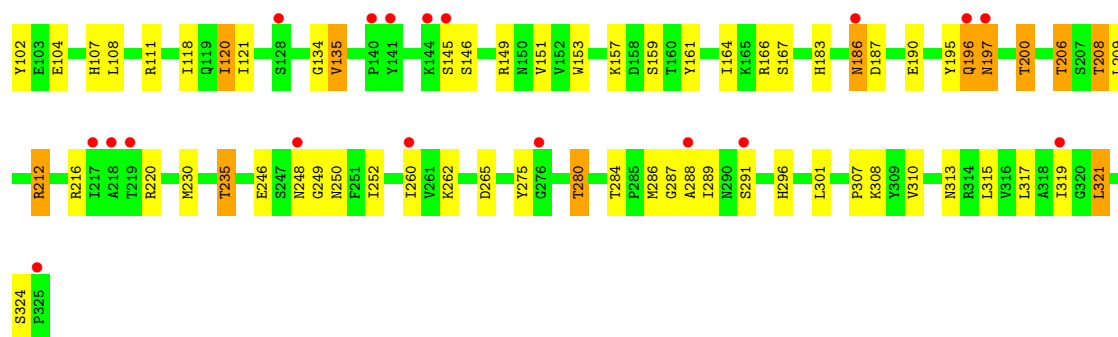


• Molecule 1: Hemagglutinin

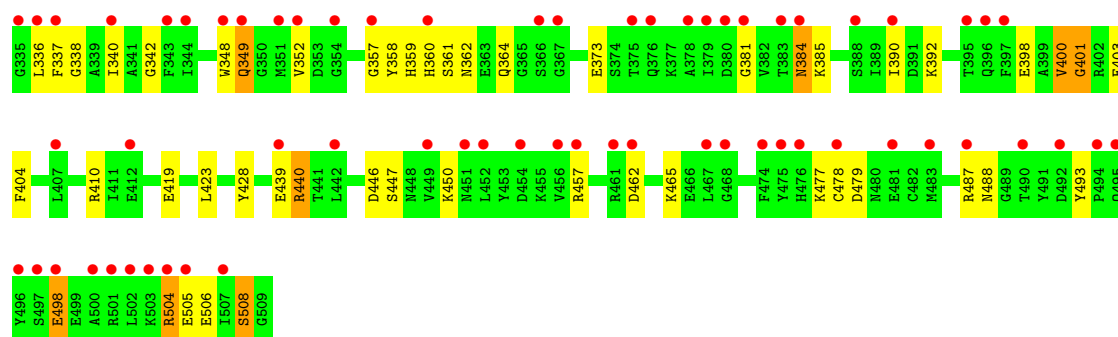


• Molecule 1: Hemagglutinin

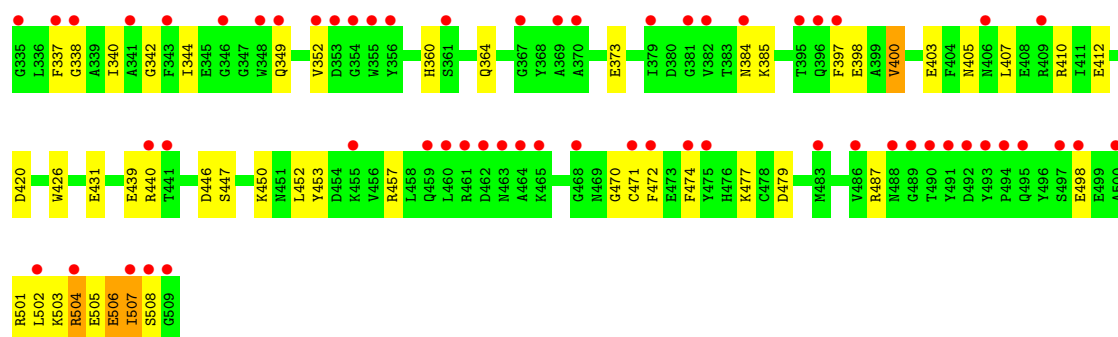




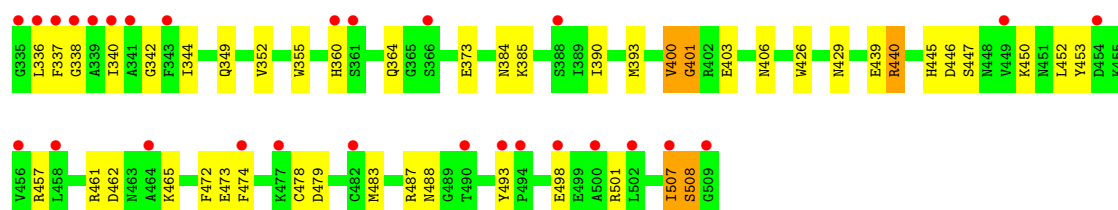
• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



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

Chain G:  100%

MAG1
MAG2

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

Chain H:  50% 50%

MAG1
MAG2

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

Chain J:  100%

MAG1
MAG2

- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  33% 67%

MAG1
GAL2
STAB

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.26Å 245.91Å 69.57Å 90.00° 112.96° 90.00°	Depositor
Resolution (Å)	34.18 – 2.40 34.18 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.2 (34.18-2.40) 97.2 (34.18-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.237 , 0.269 0.229 , 0.260	Depositor DCC
R_{free} test set	3969 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12373	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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 [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	0.61	0/2621	0.82	9/3558 (0.3%)
1	C	0.59	0/2621	0.98	10/3558 (0.3%)
1	E	0.58	0/2621	0.88	10/3558 (0.3%)
2	B	0.51	0/1443	0.62	0/1939
2	D	0.51	0/1443	0.59	0/1939
2	F	0.54	1/1443 (0.1%)	0.56	0/1939
All	All	0.57	1/12192 (0.0%)	0.80	29/16491 (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
1	A	0	1
1	C	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	429	ASN	CG-ND2	-6.90	1.15	1.32

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	57	ARG	NE-CZ-NH1	-18.41	111.10	120.30
1	C	57	ARG	NE-CZ-NH2	17.42	129.01	120.30
1	C	212	ARG	NE-CZ-NH1	-16.97	111.81	120.30
1	C	212	ARG	NE-CZ-NH2	16.17	128.38	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	149	ARG	NE-CZ-NH1	-11.93	114.34	120.30
1	E	149	ARG	NE-CZ-NH2	11.44	126.02	120.30
1	E	57	ARG	NE-CZ-NH1	10.75	125.67	120.30
1	E	57	ARG	NE-CZ-NH2	-10.68	114.96	120.30
1	A	212	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	E	212	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	C	57	ARG	CD-NE-CZ	7.38	133.94	123.60
1	A	73	GLU	C-N-CA	-7.34	103.34	121.70
1	C	212	ARG	CD-NE-CZ	7.12	133.57	123.60
1	E	212	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	A	66	LEU	N-CA-C	-6.80	92.64	111.00
1	C	149	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	E	66	LEU	N-CA-C	-6.59	93.21	111.00
1	A	212	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	73	GLU	CA-C-N	6.37	131.20	117.20
1	C	66	LEU	N-CA-C	-6.30	93.98	111.00
1	A	73	GLU	O-C-N	-6.12	112.90	122.70
1	A	57	ARG	CB-CG-CD	6.11	127.50	111.60
1	A	57	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	C	195	TYR	N-CA-C	-5.62	95.81	111.00
1	E	195	TYR	N-CA-C	-5.48	96.19	111.00
1	A	195	TYR	N-CA-C	-5.45	96.29	111.00
1	C	149	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	E	235	THR	CB-CA-C	-5.09	97.87	111.60
1	E	57	ARG	CD-NE-CZ	5.05	130.67	123.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	75	ILE	Peptide
1	C	143	GLY	Peptide
1	C	4	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	2559	0	2514	73	1
1	C	2559	0	2513	70	2
1	E	2559	0	2514	79	1
2	B	1416	0	1319	48	0
2	D	1416	0	1319	40	0
2	F	1416	0	1319	52	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
3	J	28	0	25	0	0
4	I	46	0	40	2	0
5	A	21	0	18	0	0
6	C	14	0	13	0	0
7	A	80	0	0	6	0
7	B	24	0	0	4	0
7	C	80	0	0	10	0
7	D	22	0	0	3	0
7	E	64	0	0	11	0
7	F	13	0	0	3	0
All	All	12373	0	11644	285	2

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 12.

All (285) 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:C:7:ILE:HG22	2:D:472:PHE:HB2	1.39	1.04
2:D:398:GLU:OE2	7:D:617:HOH:O	1.81	0.99
1:A:8:CYS:N	2:B:359:HIS:O	2.03	0.91
1:C:206:THR:HG22	1:C:208:THR:H	1.35	0.90
1:E:5:ASP:O	2:F:474:PHE:N	2.02	0.90
1:E:284:THR:HG22	1:E:286:MET:H	1.37	0.90
2:B:498:GLU:OE2	7:B:604:HOH:O	1.92	0.87
1:C:284:THR:HG22	1:C:286:MET:H	1.38	0.85
1:E:206:THR:HG22	1:E:208:THR:H	1.41	0.84
1:C:7:ILE:O	2:D:472:PHE:N	2.10	0.84
1:A:284:THR:HG22	1:A:286:MET:H	1.41	0.83
2:D:503:LYS:O	2:D:507:ILE:N	2.11	0.82
2:B:336:LEU:O	2:F:447:SER:OG	1.98	0.81
1:A:8:CYS:HB2	2:B:359:HIS:HB3	1.61	0.81
1:E:39:LYS:NZ	1:E:313:ASN:O	2.13	0.80
1:C:291:SER:HA	7:C:759:HOH:O	1.81	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:406:ASN:O	7:F:608:HOH:O	1.99	0.80
1:A:206:THR:HG22	1:A:208:THR:H	1.46	0.79
2:B:488:ASN:ND2	7:B:623:HOH:O	2.13	0.79
1:C:8:CYS:HA	2:D:471:CYS:HA	1.63	0.79
2:D:501:ARG:NH1	2:F:508:SER:OG	2.15	0.79
2:D:403:GLU:OE2	7:D:603:HOH:O	2.02	0.77
1:E:275:TYR:OH	7:E:557:HOH:O	2.01	0.77
1:A:8:CYS:O	2:B:359:HIS:N	2.20	0.75
1:A:39:LYS:NZ	1:A:313:ASN:O	2.16	0.74
1:C:186:ASN:O	7:C:726:HOH:O	2.04	0.74
1:E:11:TYR:OH	2:F:340:ILE:O	2.02	0.74
1:E:6:GLN:HA	2:F:472:PHE:O	1.89	0.73
1:A:200:THR:HG21	1:A:250:ASN:OD1	1.88	0.73
1:E:5:ASP:HB2	2:F:474:PHE:HB2	1.71	0.73
1:C:9:ILE:N	2:D:470:GLY:O	2.22	0.71
2:B:419:GLU:OE2	7:B:622:HOH:O	2.08	0.70
2:D:412:GLU:OE2	7:D:610:HOH:O	2.09	0.70
1:E:206:THR:HB	1:E:209:LEU:HB3	1.74	0.69
1:E:134:GLY:N	7:E:511:HOH:O	2.22	0.69
2:D:360:HIS:HD2	2:D:487:ARG:HH21	1.39	0.69
1:E:200:THR:HG21	1:E:250:ASN:OD1	1.93	0.69
2:B:360:HIS:HD2	2:B:487:ARG:HH21	1.39	0.69
2:B:360:HIS:HD2	2:B:487:ARG:NH2	1.91	0.69
1:E:85:GLU:OE2	7:E:510:HOH:O	2.10	0.68
7:C:729:HOH:O	4:I:2:GAL:O3	2.11	0.68
1:C:22:THR:HG22	1:C:24:MET:H	1.59	0.68
1:E:9:ILE:HD13	2:F:453:TYR:HA	1.75	0.68
1:E:284:THR:HB	1:E:287:GLY:O	1.95	0.67
2:D:504:ARG:O	2:D:508:SER:N	2.19	0.67
1:C:39:LYS:NZ	1:C:313:ASN:O	2.21	0.66
2:D:360:HIS:HD2	2:D:487:ARG:NH2	1.94	0.66
1:A:6:GLN:N	2:B:361:SER:O	2.25	0.66
1:A:206:THR:HB	1:A:209:LEU:HB3	1.78	0.66
1:C:200:THR:HG21	1:C:250:ASN:OD1	1.95	0.66
1:E:22:THR:HG22	1:E:24:MET:H	1.61	0.66
1:A:7:ILE:HD13	2:B:359:HIS:O	1.96	0.65
1:C:290:ASN:ND2	7:C:742:HOH:O	2.29	0.65
1:E:190:GLU:OE1	7:E:527:HOH:O	2.14	0.65
1:E:12:HIS:HB2	2:F:355:TRP:HA	1.78	0.65
2:D:501:ARG:HH12	2:F:508:SER:CB	2.09	0.65
2:B:465:LYS:NZ	2:F:461:ARG:HH12	1.95	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:HIS:ND1	2:B:403:GLU:OE1	2.26	0.64
1:A:197:ASN:N	1:A:197:ASN:OD1	2.31	0.64
1:C:301:LEU:HA	2:D:400:VAL:HG22	1.79	0.64
1:E:104:GLU:OE2	2:B:410:ARG:NE	2.26	0.64
1:A:284:THR:HB	1:A:287:GLY:O	1.99	0.63
1:E:52:LYS:HE2	7:E:557:HOH:O	1.99	0.63
2:F:488:ASN:ND2	7:F:612:HOH:O	2.29	0.63
1:E:74:PHE:HZ	1:E:76:ASN:HD22	1.47	0.62
1:C:135:VAL:HG22	1:C:146:SER:HA	1.81	0.62
1:C:284:THR:HB	1:C:287:GLY:O	2.00	0.62
1:C:197:ASN:N	1:C:197:ASN:OD1	2.33	0.62
1:A:289:ILE:HG22	1:A:291:SER:HB3	1.82	0.61
1:E:12:HIS:N	2:F:355:TRP:O	2.28	0.61
1:A:135:VAL:HG22	1:A:146:SER:HA	1.82	0.61
1:C:159:SER:O	1:C:196:GLN:HG3	2.01	0.61
1:E:301:LEU:HA	2:F:400:VAL:HG22	1.83	0.61
2:B:465:LYS:HZ3	2:F:461:ARG:HH12	1.47	0.61
1:C:206:THR:HB	1:C:209:LEU:HB3	1.82	0.60
1:A:22:THR:HG22	1:A:24:MET:H	1.67	0.60
1:C:289:ILE:HG22	1:C:291:SER:HB3	1.82	0.60
1:E:75:ILE:HG12	1:E:77:VAL:HG23	1.85	0.59
2:F:340:ILE:HG13	2:F:446:ASP:HA	1.84	0.59
1:A:197:ASN:ND2	7:A:519:HOH:O	2.36	0.58
1:C:24:MET:HA	2:B:384:ASN:HB3	1.84	0.58
1:A:5:ASP:CG	2:B:362:ASN:HA	2.23	0.58
1:C:141:TYR:CG	1:C:142:GLN:N	2.71	0.58
1:E:289:ILE:HG22	1:E:291:SER:HB3	1.84	0.58
1:A:8:CYS:O	2:B:358:TYR:HA	2.02	0.58
1:C:10:GLY:HA2	2:D:344:ILE:HG21	1.84	0.57
1:A:159:SER:O	1:A:196:GLN:HG3	2.04	0.57
1:A:99:PHE:HB3	1:A:102:TYR:HB2	1.86	0.57
1:C:7:ILE:HB	2:D:474:PHE:HE1	1.70	0.57
1:C:215:PRO:O	7:C:775:HOH:O	2.18	0.57
1:E:321:LEU:HB3	2:F:445:HIS:CD2	2.39	0.57
2:D:340:ILE:HG13	2:D:446:ASP:HA	1.86	0.56
2:D:502:LEU:O	2:D:506:GLU:HB3	2.06	0.56
2:B:340:ILE:HG13	2:B:446:ASP:HA	1.86	0.56
7:E:517:HOH:O	2:B:410:ARG:HB2	2.05	0.56
1:E:159:SER:O	1:E:196:GLN:HG3	2.05	0.56
1:E:9:ILE:O	2:F:344:ILE:HD13	2.05	0.56
1:E:99:PHE:HB3	1:E:102:TYR:HB2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:364:GLN:OE1	2:D:479:ASP:HB2	2.06	0.56
1:E:135:VAL:HG22	1:E:146:SER:HA	1.87	0.56
1:C:31:THR:HB	1:C:321:LEU:H	1.71	0.56
1:A:6:GLN:O	2:B:361:SER:N	2.36	0.55
1:C:11:TYR:OH	2:D:340:ILE:O	2.13	0.55
1:E:75:ILE:O	1:E:77:VAL:N	2.38	0.55
1:C:23:ILE:HD12	2:B:385:LYS:HG3	1.89	0.55
1:E:108:LEU:HD12	1:E:262:LYS:HD2	1.89	0.54
1:E:280:THR:HG21	1:E:288:ALA:HB1	1.88	0.54
1:C:135:VAL:HG13	1:C:145:SER:HB3	1.88	0.54
1:C:99:PHE:HB3	1:C:102:TYR:HB2	1.88	0.54
1:C:108:LEU:HD12	1:C:262:LYS:HD2	1.90	0.54
1:E:31:THR:HB	1:E:321:LEU:H	1.73	0.54
1:A:23:ILE:HD12	2:F:385:LYS:HG3	1.90	0.54
1:A:57:ARG:O	7:A:525:HOH:O	2.18	0.54
1:C:7:ILE:HB	2:D:474:PHE:CE1	2.43	0.54
1:A:120:ILE:HG22	1:A:121:ILE:HG13	1.89	0.54
1:A:301:LEU:HA	2:B:400:VAL:HG22	1.89	0.54
1:C:206:THR:HG22	1:C:209:LEU:H	1.73	0.53
1:A:108:LEU:HD12	1:A:262:LYS:HD2	1.91	0.53
1:C:280:THR:HG21	1:C:288:ALA:HB1	1.91	0.53
1:C:24:MET:HB3	2:B:381:GLY:HA2	1.92	0.52
1:A:31:THR:HB	1:A:321:LEU:H	1.74	0.52
1:E:5:ASP:N	7:E:537:HOH:O	2.35	0.52
1:E:74:PHE:CE2	1:E:76:ASN:HB2	2.45	0.52
2:B:398:GLU:OE1	2:D:420:ASP:OD2	2.28	0.52
1:A:135:VAL:HG13	1:A:145:SER:HB3	1.92	0.51
1:E:197:ASN:OD1	1:E:197:ASN:N	2.40	0.51
1:E:6:GLN:HG2	2:F:473:GLU:HA	1.91	0.51
1:E:135:VAL:HG13	1:E:145:SER:HB3	1.92	0.51
1:A:17:THR:O	7:A:575:HOH:O	2.19	0.51
1:A:206:THR:HG22	1:A:209:LEU:H	1.74	0.51
1:E:212:ARG:NH2	7:E:513:HOH:O	2.06	0.51
1:C:308:LYS:HD2	2:D:426:TRP:CE2	2.45	0.51
2:F:364:GLN:OE1	2:F:479:ASP:HB2	2.11	0.51
1:A:14:ASN:HA	2:B:349:GLN:NE2	2.26	0.51
2:B:462:ASP:OD1	2:B:493:TYR:OH	2.19	0.51
1:C:143:GLY:C	1:C:144:LYS:HG3	2.32	0.51
2:B:364:GLN:OE1	2:B:479:ASP:HB2	2.11	0.51
2:B:504:ARG:O	2:B:506:GLU:N	2.44	0.50
1:E:134:GLY:HA3	1:E:153:TRP:HB3	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:ILE:HB	2:F:474:PHE:CE1	2.47	0.50
1:C:9:ILE:HD13	2:D:453:TYR:CD1	2.45	0.50
1:C:15:ASN:OD1	1:C:15:ASN:N	2.39	0.50
2:F:478:CYS:HB3	2:F:483:MET:HE3	1.93	0.50
1:E:200:THR:OG1	1:E:248:ASN:HB3	2.11	0.49
1:E:216:ARG:O	1:E:220:ARG:NH2	2.46	0.49
1:E:161:TYR:CZ	1:E:249:GLY:HA2	2.47	0.49
2:B:337:PHE:CE1	2:B:447:SER:HB2	2.48	0.49
1:A:158:ASP:O	7:A:574:HOH:O	2.20	0.48
2:D:337:PHE:CE1	2:D:447:SER:HB2	2.48	0.48
1:A:280:THR:HG21	1:A:288:ALA:HB1	1.94	0.48
1:C:200:THR:OG1	1:C:248:ASN:HB3	2.13	0.48
1:E:107:HIS:ND1	2:F:403:GLU:OE1	2.42	0.48
1:A:161:TYR:CZ	1:A:249:GLY:HA2	2.49	0.48
2:D:504:ARG:C	2:D:506:GLU:H	2.17	0.48
2:D:360:HIS:CD2	2:D:487:ARG:NH2	2.79	0.48
1:C:161:TYR:CZ	1:C:249:GLY:HA2	2.49	0.48
1:E:68:ASN:HB3	1:E:71:CYS:SG	2.54	0.48
1:C:79:GLU:HB3	7:C:777:HOH:O	2.14	0.48
2:B:337:PHE:CE2	2:F:337:PHE:HE2	2.32	0.48
2:B:360:HIS:CD2	2:B:487:ARG:NH2	2.78	0.48
2:F:452:LEU:HD12	2:F:452:LEU:HA	1.70	0.48
1:C:23:ILE:HG22	1:C:24:MET:HG3	1.96	0.47
1:C:102:TYR:CE2	1:C:106:LYS:HD2	2.49	0.47
2:B:384:ASN:OD1	7:B:619:HOH:O	2.19	0.47
1:E:11:TYR:CZ	2:F:340:ILE:HG23	2.49	0.47
1:C:133:LEU:O	4:I:3:SIA:H113	2.14	0.47
1:E:7:ILE:HB	2:F:474:PHE:HE1	1.78	0.47
2:F:462:ASP:OD1	2:F:493:TYR:OH	2.20	0.47
1:A:164:ILE:O	1:A:246:GLU:HA	2.15	0.47
1:E:15:ASN:OD1	1:E:15:ASN:N	2.39	0.47
1:E:164:ILE:O	1:E:246:GLU:HA	2.15	0.47
1:A:309:TYR:CD2	2:B:423:LEU:HD13	2.50	0.47
1:E:23:ILE:HG22	1:E:24:MET:HG3	1.97	0.47
2:F:337:PHE:CE1	2:F:447:SER:HB2	2.50	0.46
1:E:7:ILE:HG22	2:F:472:PHE:HB2	1.97	0.46
1:C:108:LEU:CD1	1:C:262:LYS:HD2	2.46	0.46
1:E:108:LEU:CD1	1:E:262:LYS:HD2	2.46	0.46
1:E:120:ILE:HG22	1:E:121:ILE:HG13	1.97	0.46
1:C:7:ILE:HG22	2:D:472:PHE:CB	2.28	0.46
1:C:22:THR:CG2	1:C:24:MET:H	2.28	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:LYS:NZ	7:E:533:HOH:O	2.19	0.46
2:F:465:LYS:NZ	7:F:613:HOH:O	2.28	0.46
1:C:206:THR:HG22	1:C:208:THR:N	2.17	0.46
1:E:5:ASP:CG	7:E:537:HOH:O	2.54	0.46
2:F:338:GLY:O	2:F:342:GLY:HA3	2.16	0.46
1:A:15:ASN:OD1	1:A:15:ASN:N	2.38	0.46
2:B:508:SER:OG	2:F:501:ARG:NH2	2.37	0.46
1:A:36:ILE:HG22	1:A:315:LEU:CB	2.46	0.46
1:C:5:ASP:O	2:D:474:PHE:N	2.48	0.46
1:C:120:ILE:HG22	1:C:121:ILE:HG13	1.97	0.46
2:B:338:GLY:O	2:B:342:GLY:HA3	2.16	0.46
2:D:504:ARG:O	2:D:508:SER:HB3	2.16	0.45
1:A:22:THR:HG22	1:A:25:GLU:H	1.80	0.45
1:A:200:THR:OG1	1:A:248:ASN:HB3	2.16	0.45
1:E:206:THR:HG22	1:E:208:THR:N	2.20	0.45
1:E:296:HIS:CD2	1:E:307:PRO:HG2	2.51	0.45
1:A:60:SER:OG	1:A:92:ASP:HA	2.16	0.45
1:A:156:LYS:HD2	1:A:196:GLN:HG2	1.99	0.45
1:E:22:THR:CG2	1:E:24:MET:H	2.29	0.45
1:E:36:ILE:HD11	2:F:390:ILE:CG1	2.47	0.45
2:F:507:ILE:HD13	2:F:507:ILE:HA	1.69	0.45
1:A:9:ILE:C	2:B:348:TRP:CH2	2.90	0.45
2:B:428:TYR:CD1	2:F:393:MET:HA	2.52	0.45
2:B:508:SER:CB	2:F:501:ARG:HH22	2.30	0.45
1:A:159:SER:HB3	1:A:196:GLN:HE21	1.82	0.45
1:A:206:THR:HG22	1:A:208:THR:N	2.23	0.45
1:E:6:GLN:O	2:F:483:MET:HE2	2.17	0.45
1:E:7:ILE:O	2:F:472:PHE:N	2.45	0.45
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.99	0.44
1:A:36:ILE:HD11	2:B:390:ILE:HD11	1.99	0.44
1:A:108:LEU:CD1	1:A:262:LYS:HD2	2.46	0.44
1:E:183:HIS:HB2	1:E:252:ILE:HD11	1.99	0.44
1:E:206:THR:HG22	1:E:209:LEU:H	1.82	0.44
1:A:207:SER:HA	1:C:221:SER:HB2	1.99	0.44
1:C:216:ARG:NH1	7:C:716:HOH:O	2.49	0.44
1:E:321:LEU:HB3	2:F:445:HIS:CG	2.53	0.44
1:A:107:HIS:HD1	2:B:403:GLU:CD	2.15	0.44
1:C:141:TYR:HA	7:C:766:HOH:O	2.17	0.44
2:F:393:MET:HE2	2:F:393:MET:HB2	1.88	0.44
1:E:186:ASN:OD1	1:E:186:ASN:N	2.50	0.43
1:A:23:ILE:HG22	1:A:24:MET:HG3	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:291:SER:HA	7:E:508:HOH:O	2.18	0.43
1:C:321:LEU:HB2	7:C:746:HOH:O	2.18	0.43
1:A:8:CYS:C	2:B:348:TRP:HH2	2.22	0.43
1:A:120:ILE:CG2	1:A:121:ILE:HG13	2.48	0.43
1:E:308:LYS:HD2	2:F:426:TRP:CE2	2.54	0.43
1:A:144:LYS:HB3	1:A:144:LYS:HE2	1.87	0.43
1:E:23:ILE:HD12	2:D:385:LYS:HG3	2.00	0.43
2:B:400:VAL:HA	2:B:401:GLY:HA3	1.85	0.43
1:C:317:LEU:HD12	1:C:317:LEU:HA	1.79	0.43
1:A:171:THR:HA	7:A:568:HOH:O	2.19	0.43
1:A:9:ILE:HA	2:B:357:GLY:O	2.19	0.43
1:A:36:ILE:HG22	1:A:315:LEU:HB3	1.99	0.43
1:A:206:THR:CG2	1:A:207:SER:N	2.82	0.43
1:C:183:HIS:HB2	1:C:252:ILE:HD11	1.99	0.43
1:E:11:TYR:CE2	2:F:340:ILE:HA	2.54	0.43
1:E:36:ILE:HG22	1:E:315:LEU:CB	2.49	0.43
1:E:120:ILE:CG2	1:E:121:ILE:HG13	2.49	0.43
1:A:280:THR:HG22	1:A:281:LYS:H	1.83	0.42
2:B:392:LYS:HD2	2:D:431:GLU:HB3	2.01	0.42
2:D:338:GLY:O	2:D:342:GLY:HA3	2.19	0.42
2:B:440:ARG:HG3	2:F:440:ARG:NH2	2.34	0.42
2:D:405:ASN:OD1	2:D:407:LEU:N	2.43	0.42
1:A:97:GLY:HA3	1:A:230:MET:O	2.20	0.42
1:A:118:ILE:HG13	1:A:120:ILE:HD13	2.01	0.42
1:C:36:ILE:HG22	1:C:315:LEU:CB	2.50	0.42
1:C:141:TYR:CD2	1:C:142:GLN:HB2	2.54	0.42
2:D:507:ILE:HD13	2:D:507:ILE:HA	1.87	0.42
1:A:294:PRO:HG2	1:A:295:PHE:CD1	2.55	0.42
1:E:22:THR:HG22	1:E:24:MET:N	2.31	0.42
1:A:82:TYR:CE1	1:A:269:MET:HE1	2.54	0.42
1:C:9:ILE:HD13	2:D:453:TYR:HD1	1.85	0.42
2:F:360:HIS:HD2	2:F:487:ARG:HH21	1.66	0.42
1:A:102:TYR:CE2	1:A:106:LYS:HD2	2.54	0.42
1:C:22:THR:HG22	1:C:24:MET:N	2.29	0.42
1:E:36:ILE:HD11	2:F:390:ILE:HG13	2.02	0.42
2:F:400:VAL:HA	2:F:401:GLY:HA3	1.80	0.42
1:C:58:ASP:OD1	1:C:90:VAL:HG23	2.20	0.41
1:C:304:GLY:HA2	2:D:397:PHE:CD1	2.54	0.41
2:D:337:PHE:HZ	2:F:336:LEU:HB3	1.85	0.41
1:A:176:LEU:HD12	1:A:176:LEU:HA	1.97	0.41
1:E:11:TYR:HB2	1:E:321:LEU:HD11	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:LEU:CB	7:C:746:HOH:O	2.67	0.41
1:A:11:TYR:HB2	1:A:321:LEU:HD11	2.03	0.41
1:A:289:ILE:CG2	1:A:291:SER:HB3	2.50	0.41
1:C:310:VAL:CG1	1:C:312:SER:HB3	2.51	0.41
1:A:22:THR:CG2	1:A:24:MET:H	2.33	0.41
1:C:7:ILE:HD13	1:C:7:ILE:HA	1.93	0.41
1:C:294:PRO:HG2	1:C:295:PHE:CD1	2.55	0.41
1:E:97:GLY:HA3	1:E:230:MET:O	2.21	0.41
2:B:404:PHE:HA	2:D:410:ARG:NH1	2.35	0.41
2:F:508:SER:OG	2:F:508:SER:O	2.37	0.41
1:A:4:GLN:N	7:A:549:HOH:O	2.53	0.41
1:C:60:SER:OG	1:C:92:ASP:HA	2.20	0.41
1:C:281:LYS:HE2	1:C:281:LYS:HB3	1.89	0.41
1:E:118:ILE:HG13	1:E:120:ILE:HD13	2.03	0.41
2:D:452:LEU:HD12	2:D:452:LEU:HA	1.72	0.41
1:A:22:THR:HG22	1:A:24:MET:N	2.34	0.41
1:A:310:VAL:CG1	1:A:312:SER:HB3	2.51	0.40
1:C:118:ILE:HG13	1:C:120:ILE:HD13	2.02	0.40
2:B:337:PHE:CE2	2:F:337:PHE:CE2	3.09	0.40
1:A:154:LEU:O	1:A:155:ILE:HD12	2.21	0.40
1:E:9:ILE:CD1	2:F:453:TYR:HA	2.47	0.40
1:E:60:SER:OG	1:E:92:ASP:HA	2.21	0.40
1:A:68:ASN:HB3	1:A:71:CYS:SG	2.61	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:GLN:O	1:C:132:SER:OG[1_556]	2.10	0.10
1:C:58:ASP:OD2	1:E:73:GLU:OE1[1_655]	2.14	0.06

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	320/322 (99%)	300 (94%)	18 (6%)	2 (1%)	22	33
1	C	320/322 (99%)	301 (94%)	18 (6%)	1 (0%)	37	51
1	E	320/322 (99%)	302 (94%)	16 (5%)	2 (1%)	22	33
2	B	173/175 (99%)	160 (92%)	9 (5%)	4 (2%)	5	6
2	D	173/175 (99%)	162 (94%)	9 (5%)	2 (1%)	11	16
2	F	173/175 (99%)	164 (95%)	8 (5%)	1 (1%)	22	33
All	All	1479/1491 (99%)	1389 (94%)	78 (5%)	12 (1%)	16	26

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	E	74	PHE
2	B	504	ARG
2	B	508	SER
2	D	505	GLU
1	C	74	PHE
1	A	5	ASP
1	E	76	ASN
2	B	505	GLU
2	D	504	ARG
2	F	401	GLY
2	B	401	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	290/290 (100%)	257 (89%)	33 (11%)	4	6
1	C	290/290 (100%)	254 (88%)	36 (12%)	4	5
1	E	290/290 (100%)	255 (88%)	35 (12%)	4	5
2	B	149/149 (100%)	137 (92%)	12 (8%)	9	15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	149/149 (100%)	136 (91%)	13 (9%)	8	13
2	F	149/149 (100%)	137 (92%)	12 (8%)	9	15
All	All	1317/1317 (100%)	1176 (89%)	141 (11%)	5	8

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	15	ASN
1	A	16	SER
1	A	20	VAL
1	A	22	THR
1	A	23	ILE
1	A	30	VAL
1	A	31	THR
1	A	59	CYS
1	A	99	PHE
1	A	111	ARG
1	A	120	ILE
1	A	135	VAL
1	A	144	LYS
1	A	151	VAL
1	A	166	ARG
1	A	167	SER
1	A	186	ASN
1	A	187	ASP
1	A	196	GLN
1	A	197	ASN
1	A	200	THR
1	A	206	THR
1	A	208	THR
1	A	235	THR
1	A	260	ILE
1	A	265	ASP
1	A	280	THR
1	A	310	VAL
1	A	317	LEU
1	A	319	ILE
1	A	321	LEU
1	A	324	SER
1	C	7	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	15	ASN
1	C	16	SER
1	C	20	VAL
1	C	22	THR
1	C	23	ILE
1	C	30	VAL
1	C	31	THR
1	C	39	LYS
1	C	59	CYS
1	C	73	GLU
1	C	99	PHE
1	C	111	ARG
1	C	120	ILE
1	C	135	VAL
1	C	151	VAL
1	C	155	ILE
1	C	166	ARG
1	C	167	SER
1	C	186	ASN
1	C	187	ASP
1	C	196	GLN
1	C	197	ASN
1	C	200	THR
1	C	206	THR
1	C	208	THR
1	C	212	ARG
1	C	235	THR
1	C	260	ILE
1	C	265	ASP
1	C	280	THR
1	C	310	VAL
1	C	317	LEU
1	C	319	ILE
1	C	321	LEU
1	C	324	SER
1	E	4	GLN
1	E	7	ILE
1	E	15	ASN
1	E	16	SER
1	E	20	VAL
1	E	22	THR
1	E	23	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	30	VAL
1	E	31	THR
1	E	52	LYS
1	E	59	CYS
1	E	73	GLU
1	E	99	PHE
1	E	111	ARG
1	E	120	ILE
1	E	135	VAL
1	E	151	VAL
1	E	166	ARG
1	E	167	SER
1	E	186	ASN
1	E	187	ASP
1	E	196	GLN
1	E	197	ASN
1	E	200	THR
1	E	206	THR
1	E	208	THR
1	E	235	THR
1	E	260	ILE
1	E	265	ASP
1	E	280	THR
1	E	310	VAL
1	E	317	LEU
1	E	319	ILE
1	E	321	LEU
1	E	324	SER
2	B	349	GLN
2	B	352	VAL
2	B	373	GLU
2	B	384	ASN
2	B	400	VAL
2	B	439	GLU
2	B	440	ARG
2	B	450	LYS
2	B	457	ARG
2	B	477	LYS
2	B	478	CYS
2	B	498	GLU
2	D	349	GLN
2	D	352	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	373	GLU
2	D	384	ASN
2	D	400	VAL
2	D	439	GLU
2	D	440	ARG
2	D	450	LYS
2	D	457	ARG
2	D	477	LYS
2	D	498	GLU
2	D	506	GLU
2	D	507	ILE
2	F	349	GLN
2	F	352	VAL
2	F	373	GLU
2	F	384	ASN
2	F	400	VAL
2	F	439	GLU
2	F	440	ARG
2	F	450	LYS
2	F	457	ARG
2	F	498	GLU
2	F	507	ILE
2	F	508	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
1	E	76	ASN
2	B	360	HIS
2	B	396	GLN
2	B	495	GLN
2	D	360	HIS
2	D	429	ASN
2	D	495	GLN
2	F	360	HIS
2	F	396	GLN
2	F	429	ASN
2	F	495	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 ⓘ

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	3,1	14,14,15	0.65	0	17,19,21	1.09	2 (11%)
3	NAG	G	2	3	14,14,15	0.66	0	17,19,21	1.63	3 (17%)
3	NAG	H	1	3,1	14,14,15	0.51	0	17,19,21	1.11	1 (5%)
3	NAG	H	2	3	14,14,15	0.55	0	17,19,21	1.02	0
4	NAG	I	1	4	15,15,15	0.40	0	21,21,21	1.54	3 (14%)
4	GAL	I	2	4	11,11,12	1.05	1 (9%)	15,15,17	1.27	1 (6%)
4	SIA	I	3	4	20,20,21	3.50	9 (45%)	21,28,31	3.53	7 (33%)
3	NAG	J	1	3,1	14,14,15	0.51	0	17,19,21	1.19	2 (11%)
3	NAG	J	2	3	14,14,15	0.57	0	17,19,21	1.47	2 (11%)

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	-	1/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	3	SIA	C7-C6	-10.12	1.40	1.52
4	I	3	SIA	C3-C4	-6.67	1.40	1.52
4	I	3	SIA	C4-C5	-5.26	1.48	1.53
4	I	3	SIA	O4-C4	4.29	1.52	1.43
4	I	3	SIA	C3-C2	-3.97	1.46	1.52
4	I	3	SIA	O6-C6	3.18	1.48	1.44
4	I	3	SIA	O8-C8	-2.63	1.37	1.43
4	I	2	GAL	O5-C1	-2.20	1.40	1.43
4	I	3	SIA	C10-N5	2.14	1.41	1.34
4	I	3	SIA	C11-C10	2.11	1.54	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	3	SIA	O6-C2-C3	-11.54	95.04	110.56
4	I	3	SIA	O6-C2-C1	8.15	123.11	107.72
3	G	2	NAG	O5-C1-C2	-4.93	103.66	111.29
3	J	2	NAG	C2-N2-C7	-4.58	116.76	122.90
4	I	1	NAG	C1-O5-C5	4.10	121.59	113.65
4	I	3	SIA	O9-C9-C8	4.05	119.66	111.16
4	I	1	NAG	O5-C5-C4	3.60	116.19	109.70
3	G	2	NAG	C2-N2-C7	-3.33	118.44	122.90
4	I	3	SIA	O1B-C1-C2	3.26	121.20	112.71
4	I	3	SIA	C5-N5-C10	-2.84	116.45	123.11
4	I	2	GAL	C1-O5-C5	-2.75	108.50	112.19
3	G	1	NAG	C1-O5-C5	2.70	115.81	112.19
4	I	3	SIA	C11-C10-N5	2.49	120.25	116.12
4	I	3	SIA	O1B-C1-O1A	-2.49	118.43	124.08
3	J	1	NAG	C1-O5-C5	2.41	115.42	112.19
4	I	1	NAG	O5-C1-C2	2.41	111.94	109.52
3	G	2	NAG	C3-C4-C5	2.34	114.48	110.23
3	J	2	NAG	O5-C5-C6	2.32	112.17	107.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1	NAG	C2-N2-C7	-2.13	120.04	122.90
3	H	1	NAG	C1-O5-C5	-2.08	109.39	112.19
3	G	1	NAG	O4-C4-C3	-2.02	105.61	110.38

There are no chirality outliers.

All (11) torsion outliers are listed below:

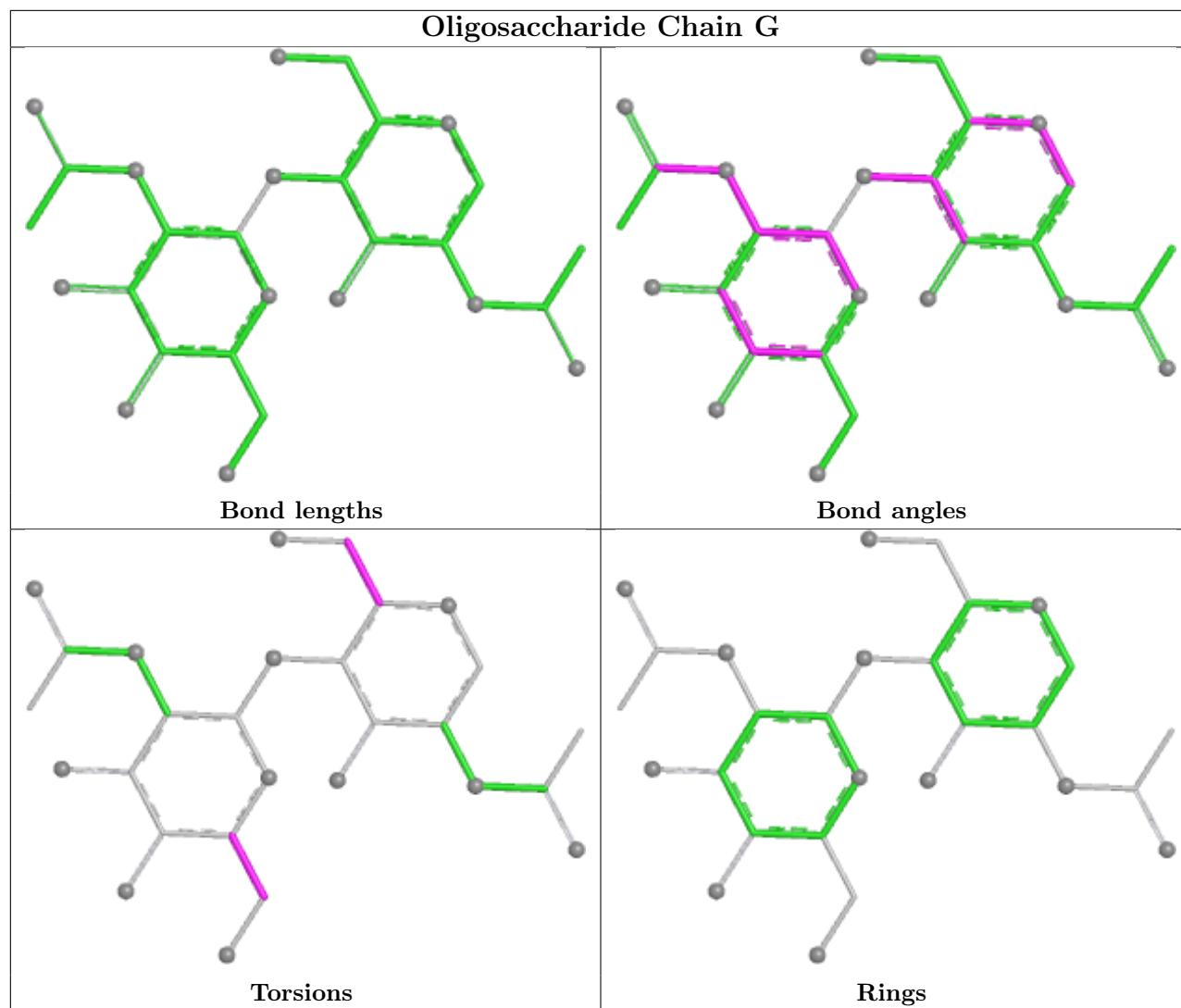
Mol	Chain	Res	Type	Atoms
4	I	1	NAG	O7-C7-N2-C2
3	J	2	NAG	C4-C5-C6-O6
4	I	2	GAL	O5-C5-C6-O6
4	I	2	GAL	C4-C5-C6-O6
4	I	1	NAG	C8-C7-N2-C2
3	J	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	J	1	NAG	C8-C7-N2-C2
3	J	1	NAG	O7-C7-N2-C2
3	G	1	NAG	C4-C5-C6-O6

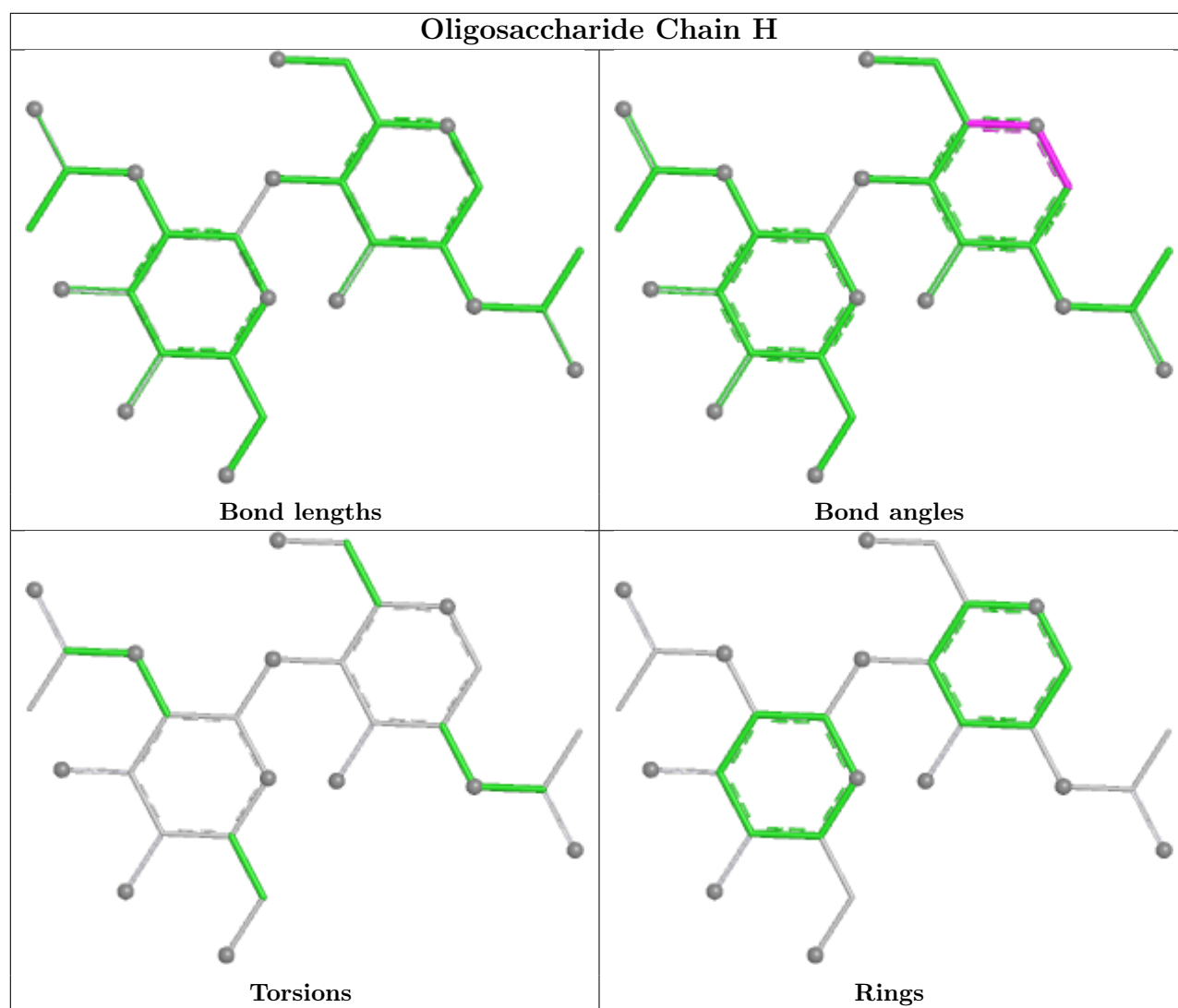
There are no ring outliers.

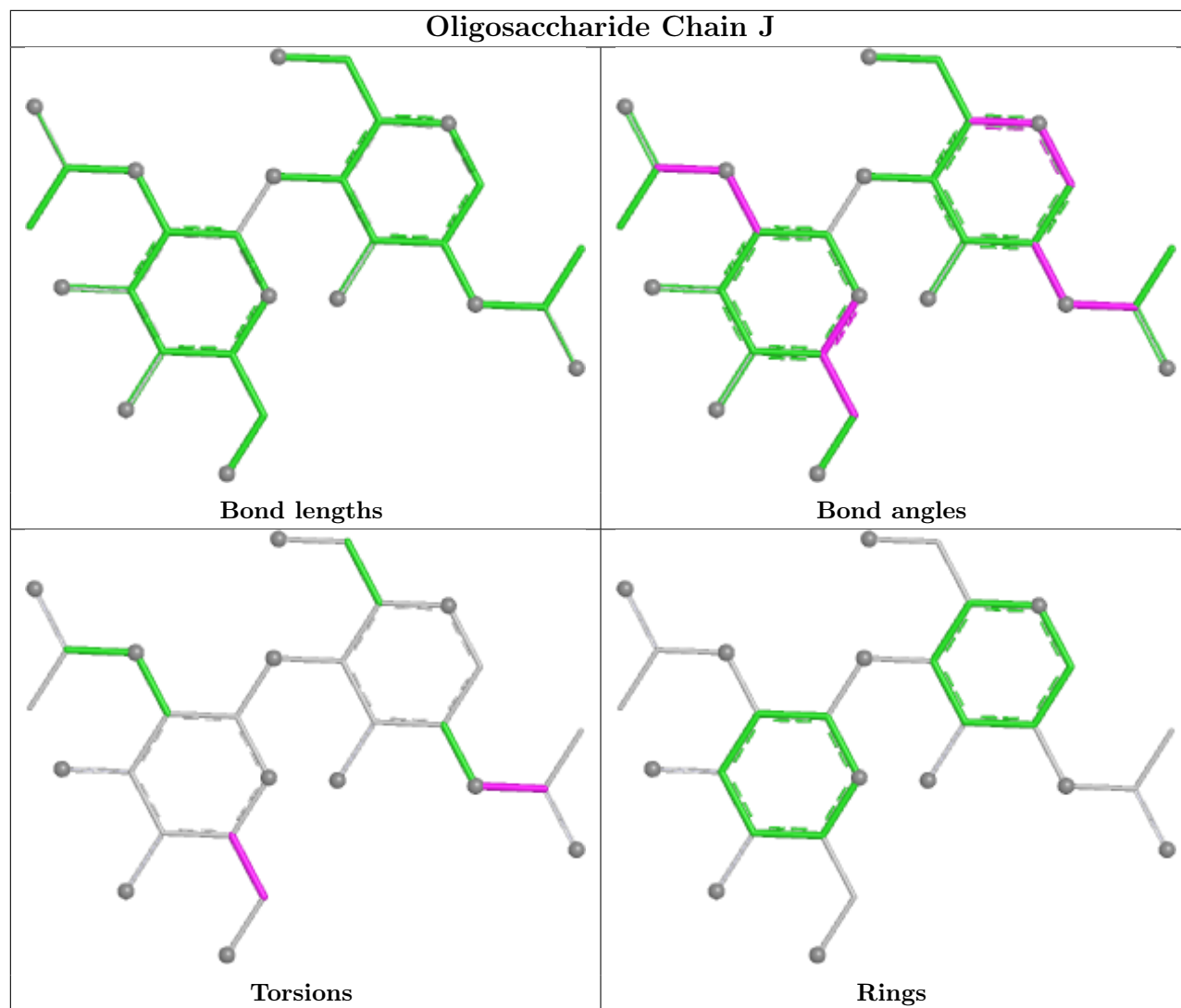
2 monomers are involved in 2 short contacts:

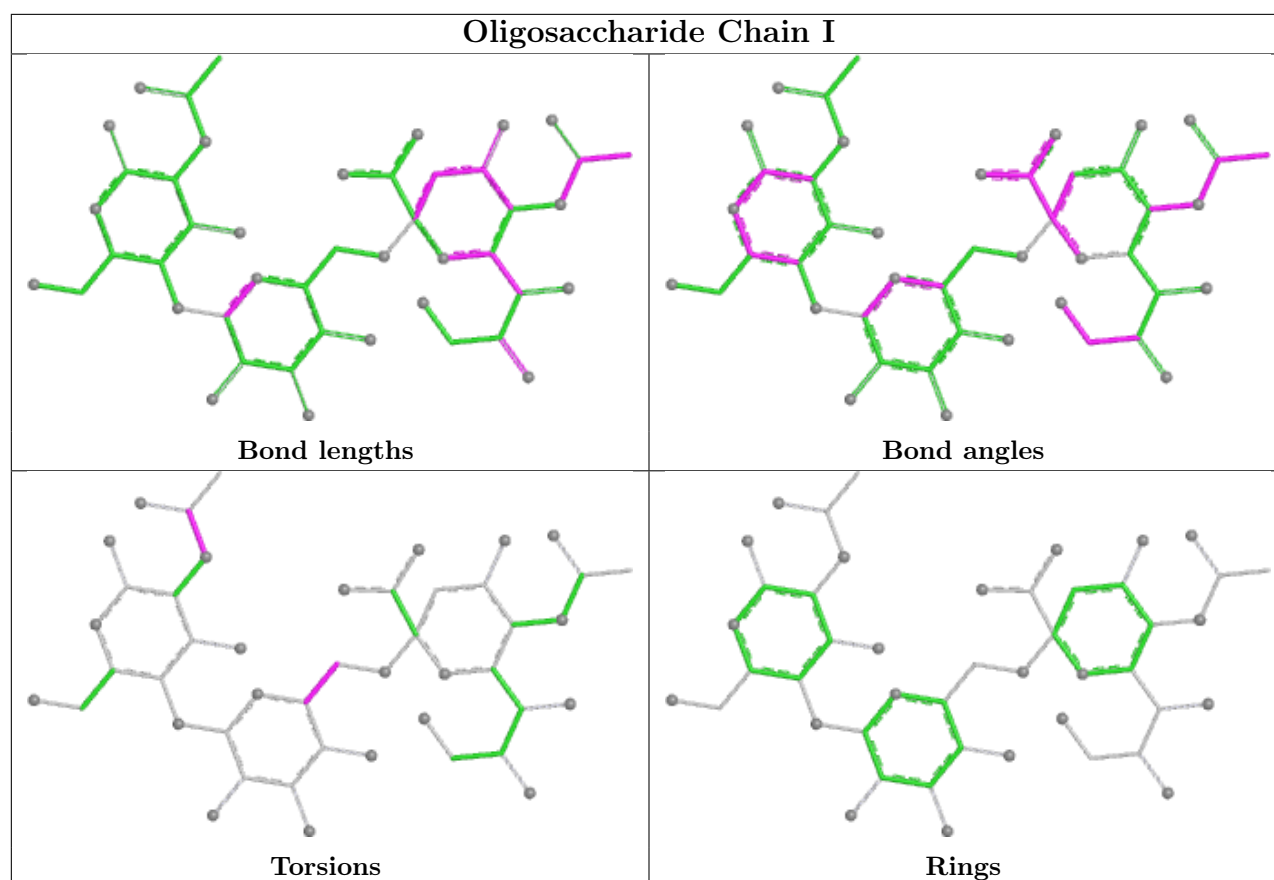
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	2	GAL	1	0
4	I	3	SIA	1	0

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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SIA	A	403	-	21,21,21	3.94	8 (38%)	24,31,31	1.97	7 (29%)
6	NAG	C	601	1	14,14,15	0.44	0	17,19,21	1.46	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	SIA	A	403	-	-	2/20/38/38	0/1/1/1
6	NAG	C	601	1	-	2/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	403	SIA	C7-C6	-9.27	1.41	1.52
5	A	403	SIA	C3-C4	-9.12	1.39	1.53
5	A	403	SIA	C4-C5	-6.88	1.47	1.53
5	A	403	SIA	O6-C6	6.02	1.53	1.44
5	A	403	SIA	O6-C2	4.67	1.47	1.43
5	A	403	SIA	C3-C2	-4.21	1.46	1.51
5	A	403	SIA	O4-C4	3.96	1.51	1.43
5	A	403	SIA	O8-C8	-2.01	1.39	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	601	NAG	C1-O5-C5	5.13	119.06	112.19
5	A	403	SIA	O6-C6-C7	4.76	114.09	106.65
5	A	403	SIA	C6-C5-N5	-4.01	104.50	110.91
5	A	403	SIA	C8-C7-C6	-3.02	107.39	113.05
5	A	403	SIA	O6-C6-C5	-2.71	107.37	109.84
5	A	403	SIA	O4-C4-C3	2.56	115.93	109.97
5	A	403	SIA	C3-C4-C5	2.36	113.36	109.72
5	A	403	SIA	O7-C7-C6	2.15	114.09	109.44

There are no chirality outliers.

All (4) torsion outliers are listed below:

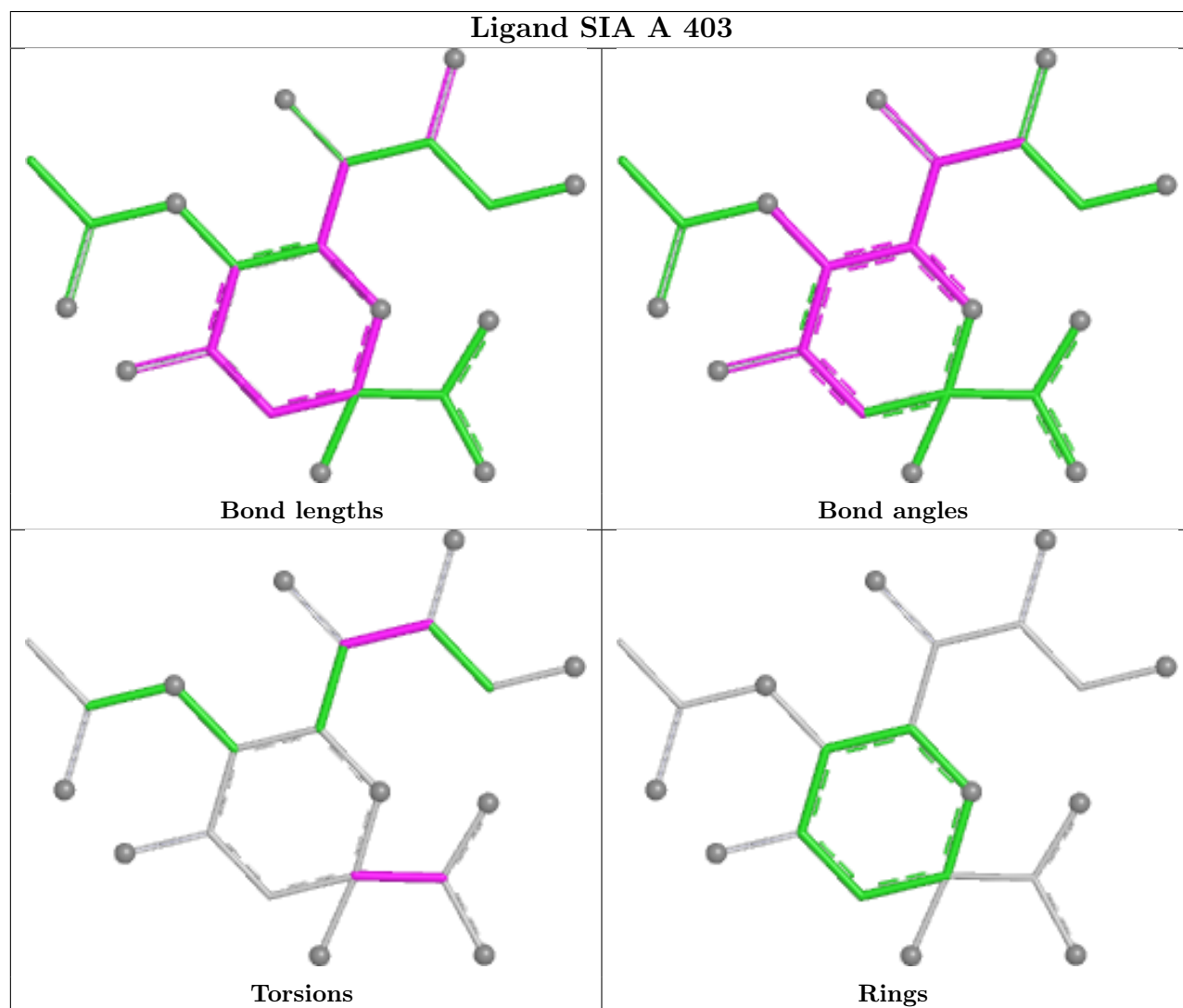
Mol	Chain	Res	Type	Atoms
6	C	601	NAG	O7-C7-N2-C2
6	C	601	NAG	C8-C7-N2-C2
5	A	403	SIA	C6-C7-C8-O8
5	A	403	SIA	O1B-C1-C2-C3

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 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 [i](#)

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(Å ²)	Q < 0.9
1	A	322/322 (100%)	0.53	35 (10%)	12 10	24, 48, 89, 162	0
1	C	322/322 (100%)	0.69	35 (10%)	12 10	26, 51, 96, 150	0
1	E	322/322 (100%)	0.80	38 (11%)	10 9	27, 54, 103, 167	0
2	B	175/175 (100%)	1.67	63 (36%)	1 1	34, 78, 126, 170	0
2	D	175/175 (100%)	1.54	59 (33%)	1 1	31, 92, 146, 183	0
2	F	175/175 (100%)	1.00	28 (16%)	6 5	32, 90, 143, 205	0
All	All	1491/1491 (100%)	0.93	258 (17%)	5 5	24, 58, 126, 205	0

All (258) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	141	TYR	8.1
1	C	141	TYR	6.5
1	A	7	ILE	6.3
2	F	482	CYS	6.1
1	C	5	ASP	5.5
1	C	144	LYS	5.4
1	E	7	ILE	5.4
1	E	75	ILE	5.3
1	E	31	THR	5.0
2	B	502	LEU	5.0
1	E	217	ILE	4.9
1	E	74	PHE	4.8
1	E	10	GLY	4.8
2	D	507	ILE	4.7
2	D	335	GLY	4.7
1	A	290	ASN	4.6
2	B	501	ARG	4.6
2	B	498	GLU	4.6
1	A	291	SER	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	5	ASP	4.5
2	B	504	ARG	4.4
2	B	388	SER	4.4
2	F	509	GLY	4.4
1	A	72	ASP	4.3
2	D	353	ASP	4.3
2	D	395	THR	4.3
2	B	497	SER	4.3
2	B	490	THR	4.2
2	B	348	TRP	4.2
1	E	13	ALA	4.0
1	E	71	CYS	3.9
2	D	508	SER	3.9
1	E	8	CYS	3.8
1	C	70	MET	3.8
1	A	218	ALA	3.8
2	D	381	GLY	3.8
2	D	490	THR	3.8
2	B	500	ALA	3.7
1	C	143	GLY	3.7
2	D	370	ALA	3.7
2	D	475	TYR	3.7
1	E	5	ASP	3.7
1	E	9	ILE	3.6
1	E	70	MET	3.6
1	C	7	ILE	3.6
2	F	343	PHE	3.6
2	D	502	LEU	3.6
2	D	337	PHE	3.5
2	F	337	PHE	3.5
1	C	73	GLU	3.5
1	E	218	ALA	3.5
2	B	407	LEU	3.5
2	B	451	ASN	3.5
2	D	509	GLY	3.5
1	C	126	TRP	3.4
1	A	16	SER	3.4
2	B	494	PRO	3.4
2	F	474	PHE	3.3
1	A	278	CYS	3.3
1	E	186	ASN	3.3
1	A	8	CYS	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	465	LYS	3.3
1	E	128	SER	3.3
2	D	384	ASN	3.3
1	E	276	GLY	3.2
1	A	120	ILE	3.2
2	B	375	THR	3.2
2	B	343	PHE	3.2
1	A	32	HIS	3.2
2	B	367	GLY	3.2
2	B	395	THR	3.2
1	E	197	ASN	3.1
2	B	351	MET	3.1
2	D	494	PRO	3.1
1	A	323	ASN	3.1
2	B	380	ASP	3.1
1	A	6	GLN	3.1
2	D	346	GLY	3.1
1	C	127	SER	3.1
1	E	144	LYS	3.1
2	D	396	GLN	3.0
2	B	503	LYS	3.0
2	B	354	GLY	3.0
1	E	291	SER	3.0
2	F	366	SER	3.0
1	E	325	PRO	3.0
1	A	9	ILE	3.0
2	D	492	ASP	3.0
2	D	341	ALA	3.0
2	F	449	VAL	2.9
2	B	396	GLN	2.9
2	B	483	MET	2.9
2	B	397	PHE	2.9
2	B	335	GLY	2.9
2	D	468	GLY	2.9
2	F	507	ILE	2.9
2	B	378	ALA	2.9
2	D	343	PHE	2.8
2	F	361	SER	2.8
1	C	158	ASP	2.8
2	D	369	ALA	2.8
2	D	441	THR	2.8
2	B	507	ILE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	488	ASN	2.8
2	D	493	TYR	2.8
1	A	10	GLY	2.8
1	C	217	ILE	2.8
1	A	324	SER	2.8
1	A	58	ASP	2.8
2	B	492	ASP	2.8
2	D	409	ARG	2.8
2	D	440	ARG	2.8
2	B	468	GLY	2.7
2	F	338	GLY	2.7
1	C	29	THR	2.7
1	E	140	PRO	2.7
1	C	225	GLY	2.7
2	B	452	LEU	2.7
2	D	379	ILE	2.7
1	C	132	SER	2.7
2	B	454	ASP	2.7
2	B	442	LEU	2.7
1	A	186	ASN	2.7
2	D	464	ALA	2.7
2	B	366	SER	2.6
2	F	477	LYS	2.6
2	B	496	TYR	2.6
2	D	338	GLY	2.6
1	A	127	SER	2.6
1	C	137	SER	2.6
2	F	335	GLY	2.6
2	F	336	LEU	2.6
1	C	31	THR	2.6
2	F	493	TYR	2.6
1	C	4	GLN	2.6
2	D	459	GLN	2.6
2	D	500	ALA	2.5
1	E	248	ASN	2.5
1	C	9	ILE	2.5
2	B	360	HIS	2.5
1	C	79	GLU	2.5
1	A	13	ALA	2.5
2	F	360	HIS	2.5
2	F	340	ILE	2.5
2	D	361	SER	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	495	GLN	2.5
1	A	319	ILE	2.5
1	E	36	ILE	2.5
2	B	449	VAL	2.5
2	B	467	LEU	2.5
1	C	324	SER	2.4
2	D	498	GLU	2.4
2	B	357	GLY	2.4
2	D	460	LEU	2.4
1	E	219	THR	2.4
1	C	291	SER	2.4
2	B	481	GLU	2.4
2	B	505	GLU	2.4
2	D	455	LYS	2.4
1	C	76	ASN	2.4
2	B	456	VAL	2.4
2	B	383	THR	2.4
1	C	145	SER	2.4
1	E	11	TYR	2.4
2	B	478	CYS	2.4
1	E	33	ALA	2.4
2	F	502	LEU	2.4
2	D	348	TRP	2.4
2	D	397	PHE	2.4
2	B	412	GLU	2.4
2	B	462	ASP	2.4
2	B	475	TYR	2.4
2	B	461	ARG	2.4
2	D	461	ARG	2.4
1	E	90	VAL	2.3
2	B	352	VAL	2.3
2	D	352	VAL	2.3
1	A	70	MET	2.3
2	B	340	ILE	2.3
1	C	15	ASN	2.3
1	C	30	VAL	2.3
1	C	36	ILE	2.3
2	B	379	ILE	2.3
2	D	504	ARG	2.3
2	B	384	ASN	2.3
2	D	382	VAL	2.3
1	A	74	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	355	TRP	2.3
2	D	497	SER	2.3
2	D	489	GLY	2.3
1	C	33	ALA	2.3
2	F	339	ALA	2.3
2	F	454	ASP	2.3
1	A	11	TYR	2.2
1	A	141	TYR	2.2
2	D	463	ASN	2.2
2	F	464	ALA	2.2
1	A	31	THR	2.2
2	F	494	PRO	2.2
1	E	12	HIS	2.2
2	B	349	GLN	2.2
1	A	265	ASP	2.2
2	B	344	ILE	2.2
2	F	341	ALA	2.2
1	A	280	THR	2.2
2	D	471	CYS	2.2
2	D	367	GLY	2.2
1	A	76	ASN	2.2
2	B	336	LEU	2.2
2	B	487	ARG	2.2
2	F	458	LEU	2.2
1	C	13	ALA	2.2
1	E	196	GLN	2.2
2	D	495	GLN	2.2
2	B	439	GLU	2.2
2	B	457	ARG	2.2
1	A	188	ALA	2.2
2	B	376	GLN	2.2
1	C	90	VAL	2.2
2	D	486	VAL	2.2
2	F	388	SER	2.1
2	F	498	GLU	2.1
1	E	76	ASN	2.1
1	A	325	PRO	2.1
2	F	490	THR	2.1
2	F	456	VAL	2.1
2	B	474	PHE	2.1
2	D	483	MET	2.1
1	E	72	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	381	GLY	2.1
2	B	476	HIS	2.1
2	D	349	GLN	2.1
2	D	462	ASP	2.1
1	E	145	SER	2.1
1	C	240	ASN	2.1
2	F	500	ALA	2.1
2	D	356	TYR	2.1
1	A	57	ARG	2.1
2	B	337	PHE	2.1
2	D	472	PHE	2.1
1	C	10	GLY	2.1
1	E	260	ILE	2.1
1	E	319	ILE	2.1
1	C	196	GLN	2.1
1	E	6	GLN	2.1
1	A	12	HIS	2.0
2	B	390	ILE	2.0
2	D	406	ASN	2.0
1	E	29	THR	2.0
1	E	288	ALA	2.0
2	D	474	PHE	2.0
2	D	491	TYR	2.0
1	C	72	ASP	2.0
2	D	354	GLY	2.0
1	A	36	ILE	2.0
1	A	248	ASN	2.0
1	C	325	PRO	2.0
1	C	8	CYS	2.0

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

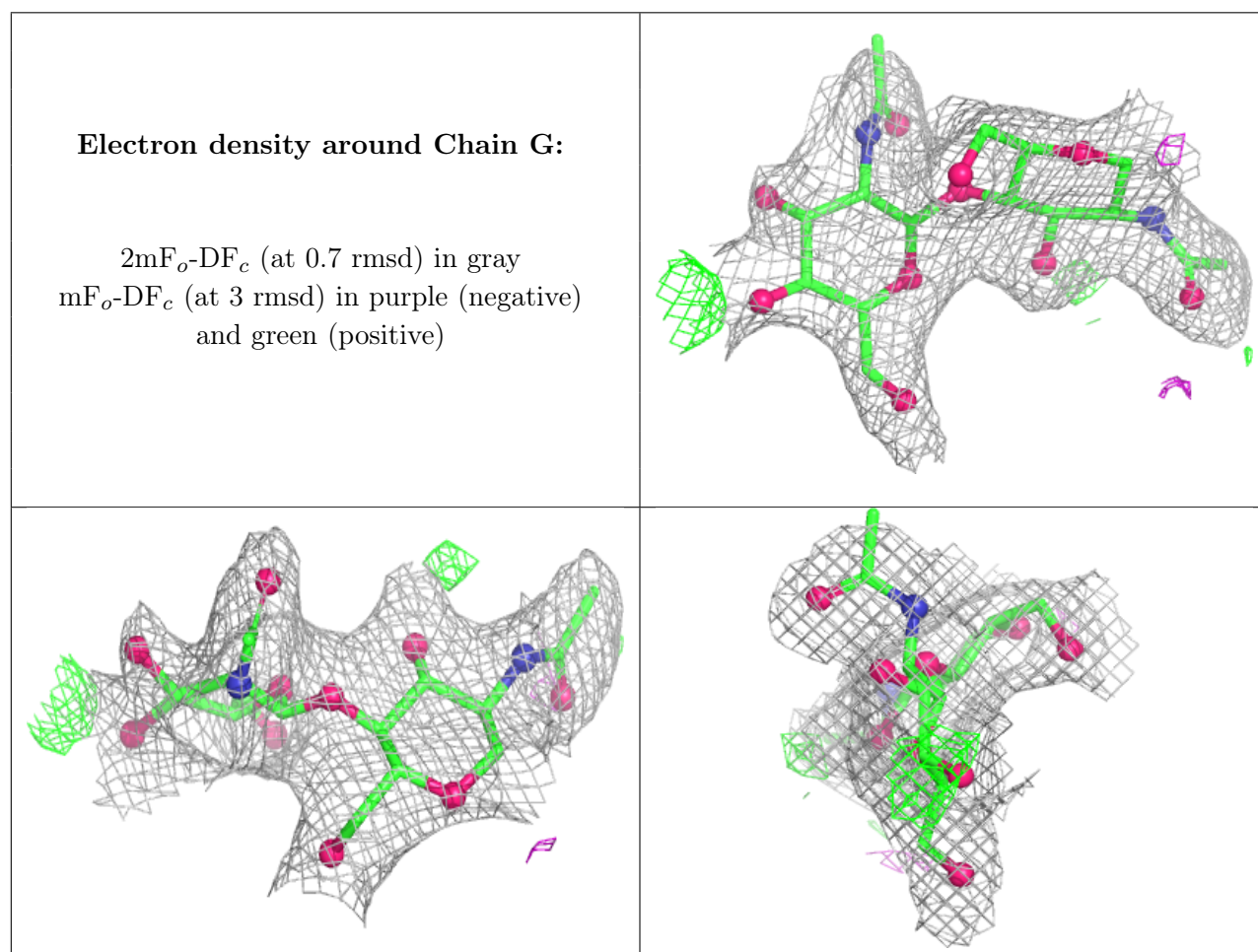
There are no non-standard protein/DNA/RNA residues in this entry.

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.

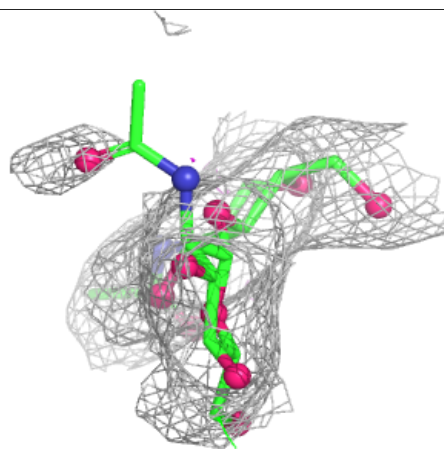
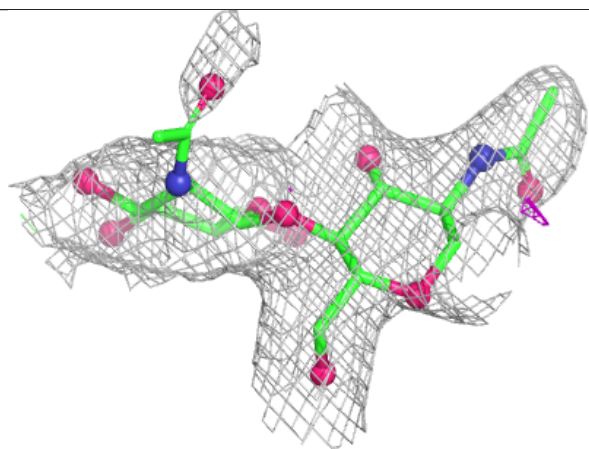
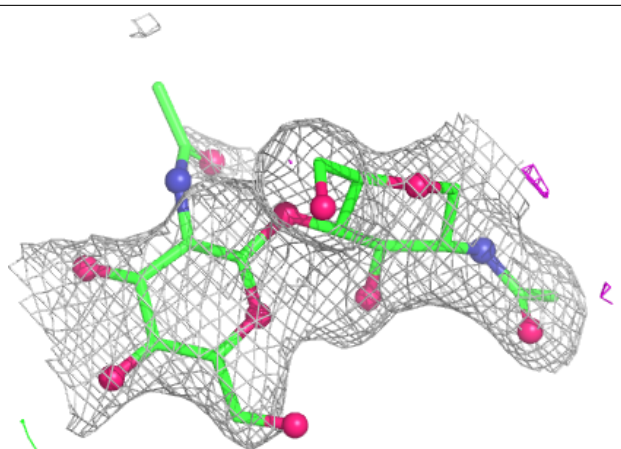
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	I	1	15/15	0.67	0.15	119,129,140,147	0
3	NAG	H	2	14/15	0.75	0.13	86,97,111,112	0
3	NAG	G	2	14/15	0.81	0.11	65,79,88,93	0
4	GAL	I	2	11/12	0.82	0.10	81,96,111,112	0
3	NAG	J	2	14/15	0.83	0.12	85,107,117,122	0
3	NAG	H	1	14/15	0.86	0.11	55,68,85,86	0
3	NAG	G	1	14/15	0.89	0.09	37,50,65,67	0
3	NAG	J	1	14/15	0.91	0.10	45,58,69,75	0
4	SIA	I	3	20/21	0.91	0.11	46,60,74,74	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.



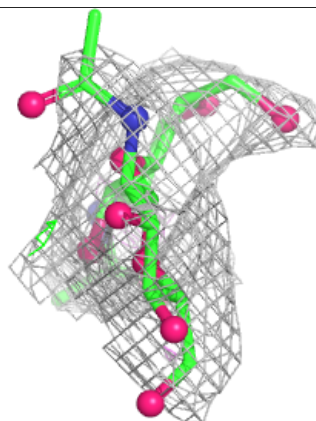
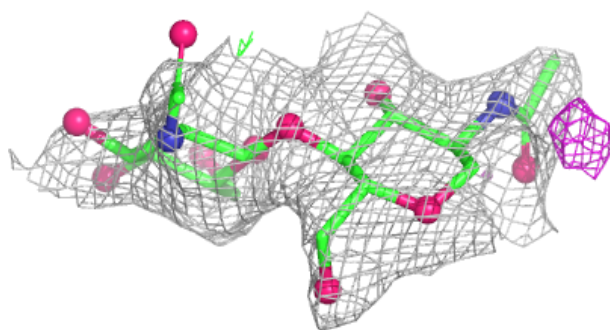
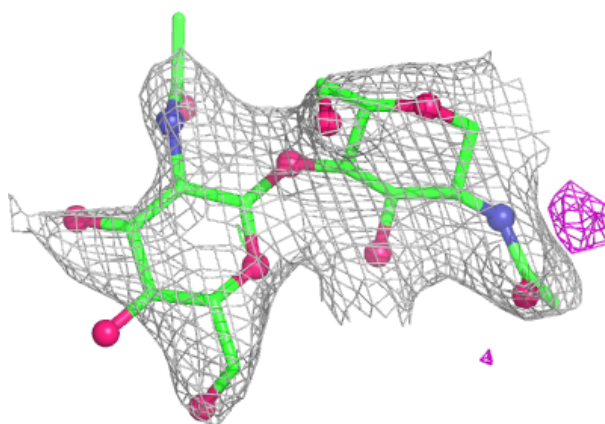
Electron density around Chain H:

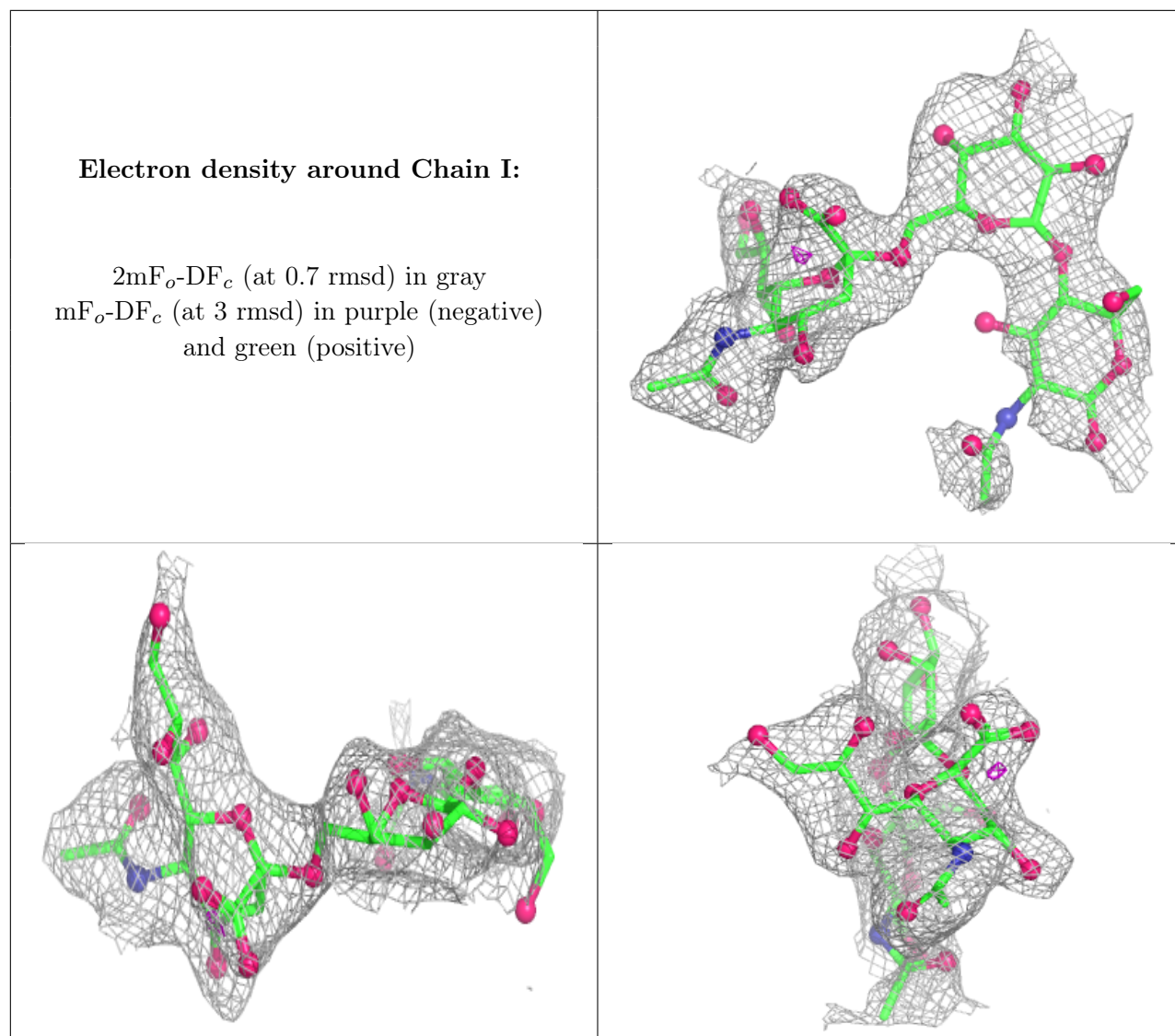
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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 ⓘ

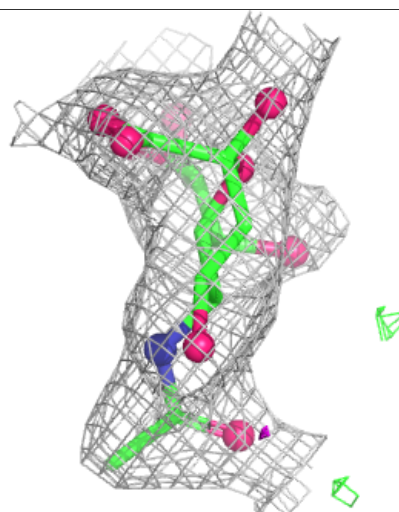
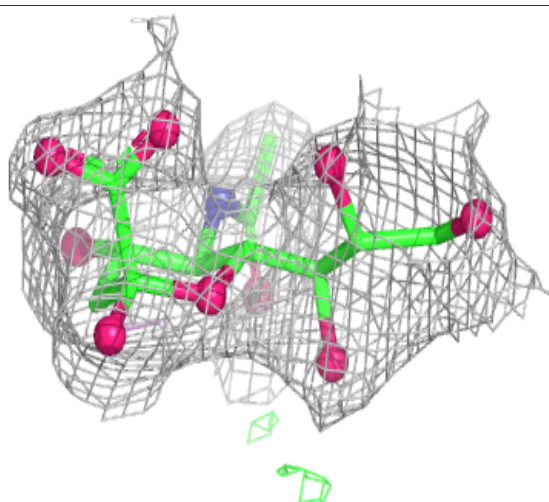
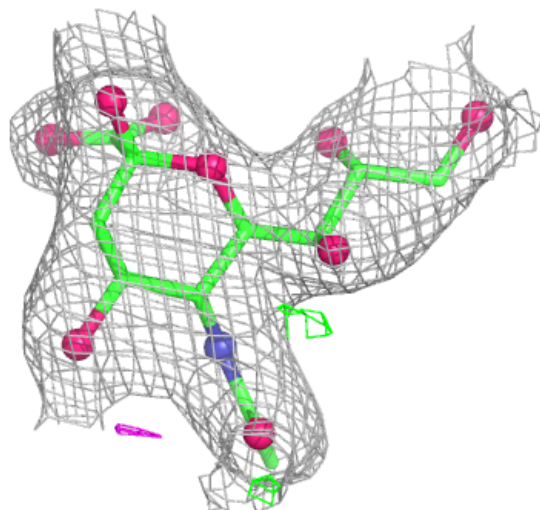
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NAG	C	601	14/15	0.67	0.15	98,114,123,128	0
5	SIA	A	403	21/21	0.89	0.11	51,57,68,69	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.

Electron density around SIA A 403:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.