



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:45 PM UTC

PDB ID : 5HMG / pdb_00005hmg
Title : REFINEMENT OF THE INFLUENZA VIRUS HEMAGGLUTININ BY SIMULATED ANNEALING
Authors : Weis, W.I.; Bruenger, A.T.; Skehel, J.J.; Wiley, D.C.
Deposited on : 1989-09-11
Resolution : 3.20 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

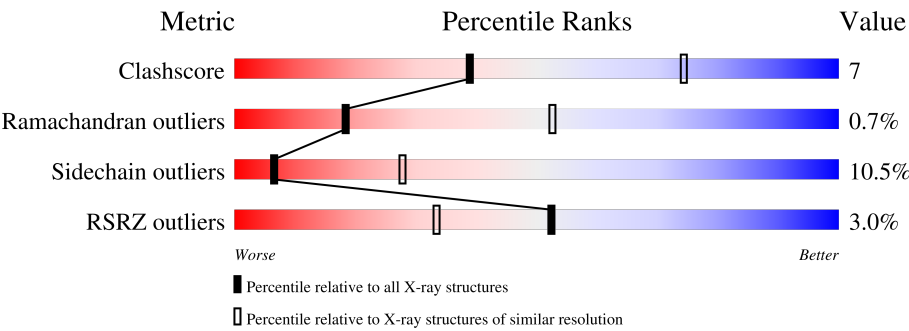
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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.



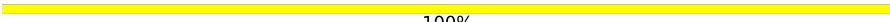
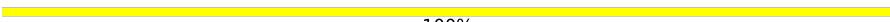
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	328	3% 70% 24% 6%
1	C	328	5% 71% 22% 6% .
1	E	328	3% 69% 25% 5%
2	B	175	2% 64% 29% 5% .
2	D	175	% 65% 30% . .
2	F	175	2% 67% 28% . .
3	G	3	100%

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Mol	Chain	Length	Quality of chain
3	H	3	 100%
3	I	3	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MAN	G	3	X	-	-	-
3	MAN	H	3	X	-	-	-
3	MAN	I	3	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12234 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	328	Total	C	N	O	S	0	0	0
			2532	1581	445	493	13			
1	C	328	Total	C	N	O	S	0	0	0
			2532	1581	445	493	13			
1	E	328	Total	C	N	O	S	0	0	0
			2532	1581	445	493	13			

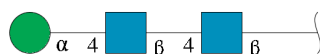
- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1417	880	250	281	6			
2	D	175	Total	C	N	O	S	0	0	0
			1417	880	250	281	6			
2	F	175	Total	C	N	O	S	0	0	0
			1417	880	250	281	6			

There are 3 discrepancies between the modelled and reference sequences:

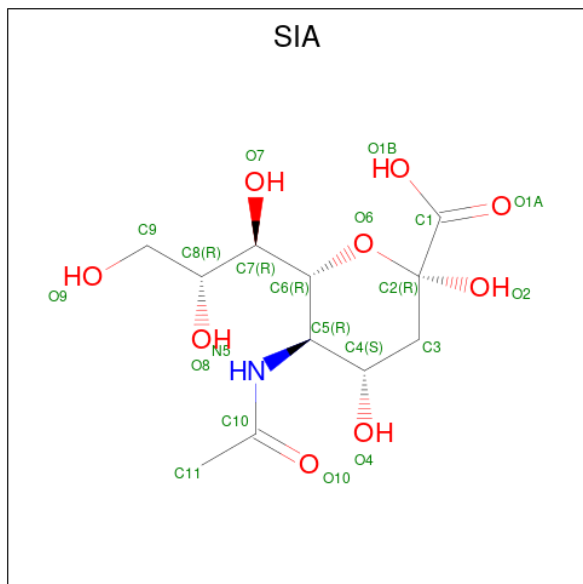
Chain	Residue	Modelled	Actual	Comment	Reference
B	112	GLY	ASP	conflict	UNP P03437
D	112	GLY	ASP	conflict	UNP P03437
F	112	GLY	ASP	conflict	UNP P03437

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



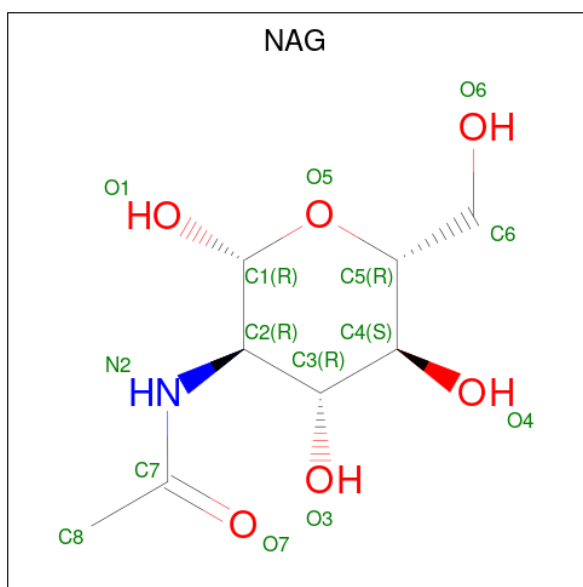
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is N-acetyl-alpha-neuraminic acid (CCD ID: SIA) (formula: $C_{11}H_{19}NO_9$).



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

- 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	A	1	Total	C	N	O	0	0
			14	8	1	5		
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	C	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	E	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		

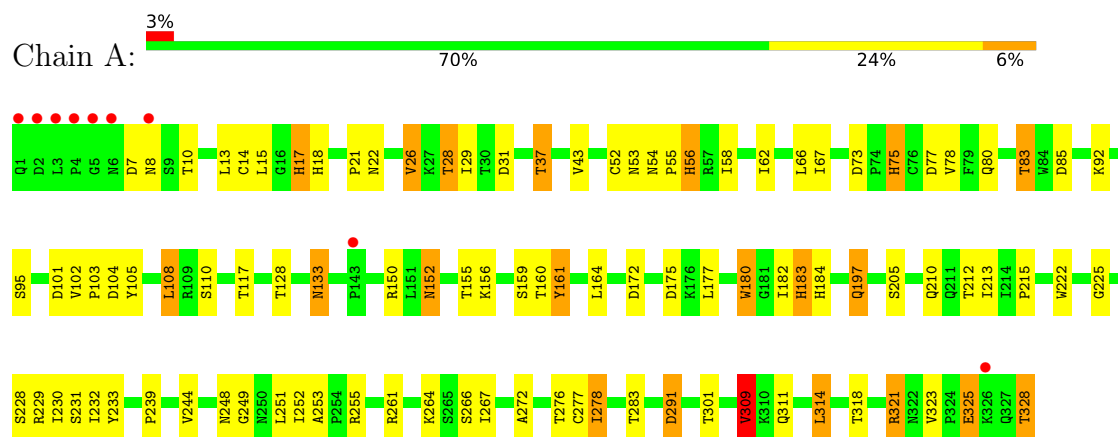
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total 8	O 8	0	0
6	B	5	Total 5	O 5	0	0
6	C	8	Total 8	O 8	0	0
6	D	5	Total 5	O 5	0	0
6	E	9	Total 9	O 9	0	0
6	F	4	Total 4	O 4	0	0

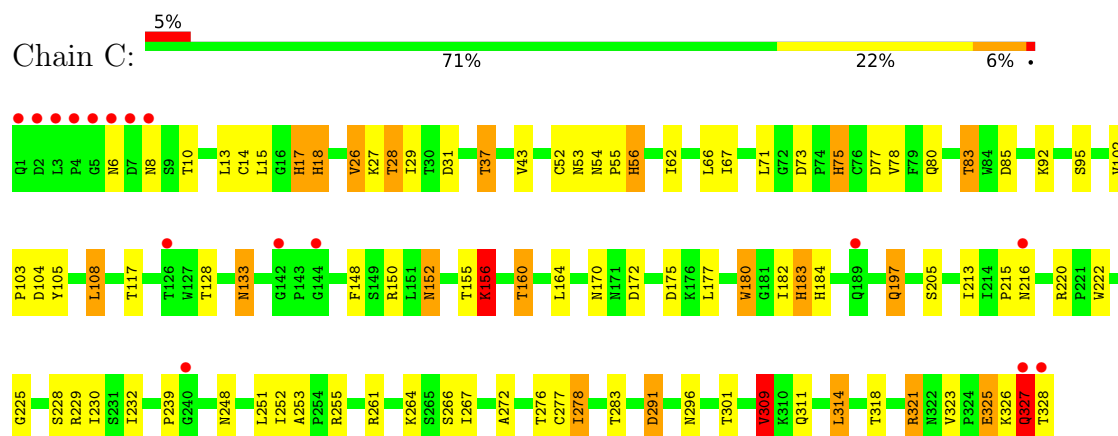
3 Residue-property plots [i](#)

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.

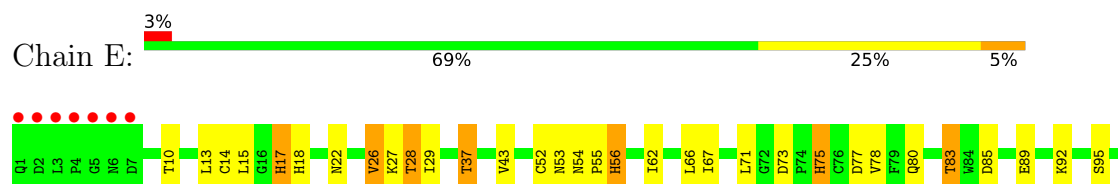
- Molecule 1: Hemagglutinin HA1 chain

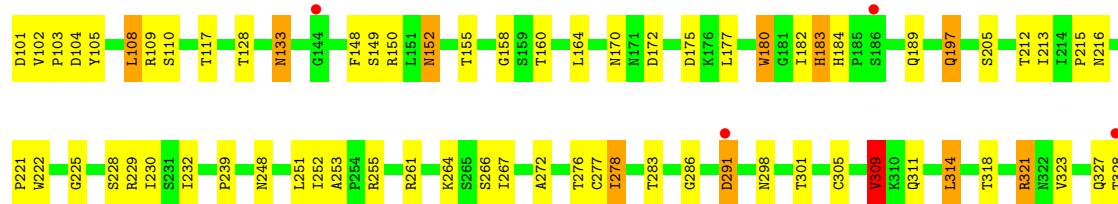


- Molecule 1: Hemagglutinin HA1 chain

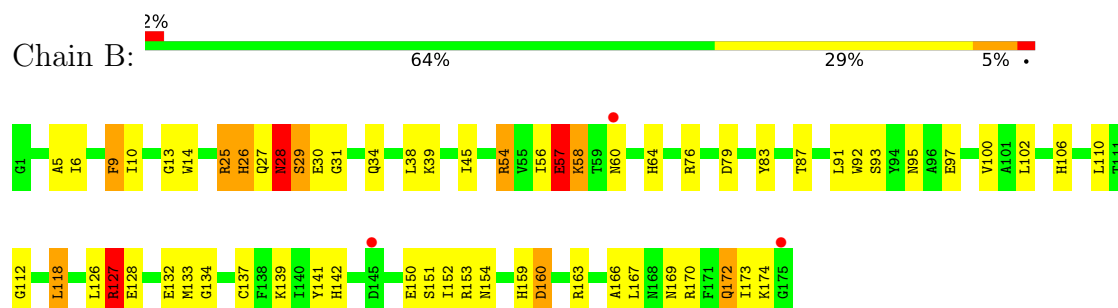


- Molecule 1: Hemagglutinin HA1 chain

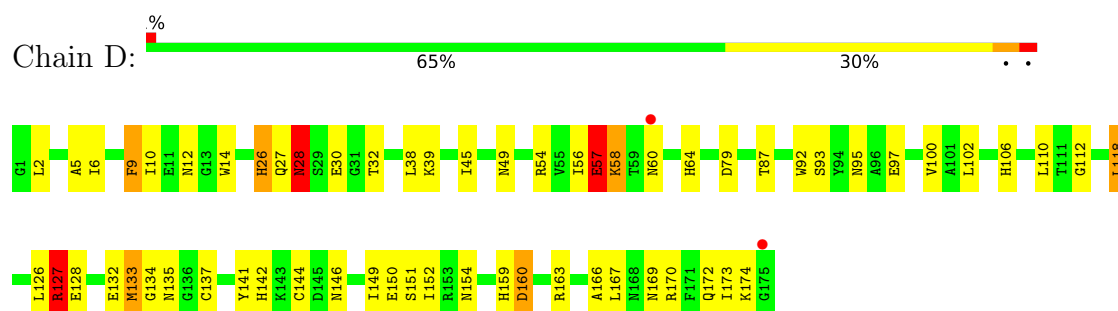




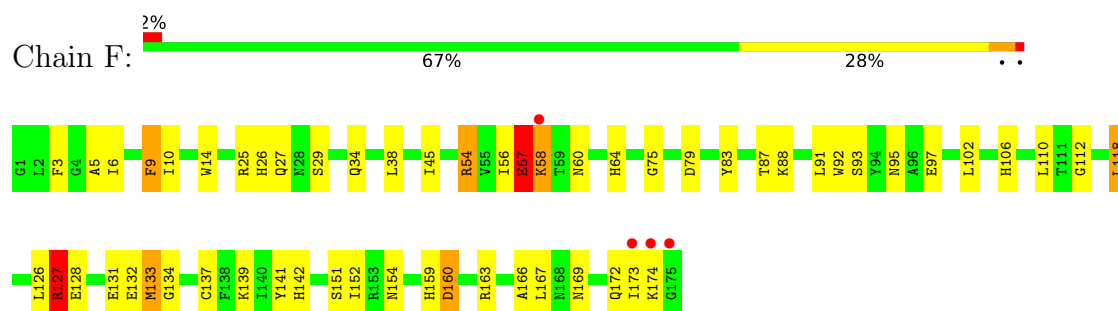
• Molecule 2: Hemagglutinin HA2 chain



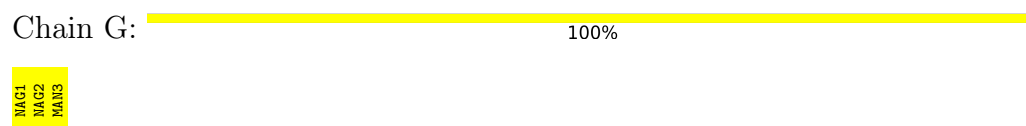
• Molecule 2: Hemagglutinin HA2 chain



• Molecule 2: Hemagglutinin HA2 chain



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



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

Chain H:  100%

MAG1
MAG2
MAN3

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

Chain I:  100%

MAG1
MAG2
MAN3

4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	162.60Å 162.60Å 177.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.20 162.60 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-3.20) 71.2 (162.60-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.220 , (Not available) 0.207 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 51.4	EDS
L-test for twinning ¹	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.056 for h,-k,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	12234	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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: NAG, SIA, MAN

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	1.07	7/2589 (0.3%)	1.72	45/3527 (1.3%)
1	C	1.09	8/2589 (0.3%)	1.73	44/3527 (1.2%)
1	E	1.11	10/2589 (0.4%)	1.70	43/3527 (1.2%)
2	B	1.10	8/1441 (0.6%)	1.72	24/1933 (1.2%)
2	D	1.15	8/1441 (0.6%)	1.74	22/1933 (1.1%)
2	F	1.12	9/1441 (0.6%)	1.73	23/1933 (1.2%)
All	All	1.10	50/12090 (0.4%)	1.72	201/16380 (1.2%)

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	106	HIS	CD2-NE2	-7.75	1.29	1.37
1	E	184	HIS	CD2-NE2	-7.14	1.29	1.37
1	E	56	HIS	CD2-NE2	-7.13	1.30	1.37
1	C	184	HIS	CD2-NE2	-7.10	1.30	1.37
1	C	56	HIS	CD2-NE2	-7.02	1.30	1.37
2	F	159	HIS	CG-ND1	-6.93	1.30	1.38
2	F	106	HIS	CD2-NE2	-6.89	1.30	1.37
2	B	159	HIS	CG-ND1	-6.82	1.30	1.38
2	F	159	HIS	CD2-NE2	-6.82	1.30	1.37
1	C	75	HIS	CD2-NE2	-6.62	1.30	1.37
1	E	17	HIS	CD2-NE2	-6.59	1.30	1.37
1	A	56	HIS	CD2-NE2	-6.54	1.30	1.37
2	D	26	HIS	CD2-NE2	-6.53	1.30	1.37
1	E	75	HIS	CD2-NE2	-6.42	1.30	1.37
1	A	17	HIS	CD2-NE2	-6.38	1.30	1.37
2	F	64	HIS	CD2-NE2	-6.36	1.30	1.37
2	D	106	HIS	CG-ND1	-6.33	1.31	1.38
1	C	17	HIS	CD2-NE2	-6.30	1.30	1.37
2	D	142	HIS	CD2-NE2	-6.25	1.30	1.37
2	F	26	HIS	CD2-NE2	-6.24	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	159	HIS	CG-ND1	-6.22	1.31	1.38
2	B	159	HIS	CD2-NE2	-6.21	1.31	1.37
1	A	75	HIS	CD2-NE2	-6.19	1.31	1.37
1	A	184	HIS	CD2-NE2	-6.06	1.31	1.37
1	E	184	HIS	CG-ND1	-5.97	1.31	1.38
1	C	75	HIS	CG-ND1	-5.88	1.31	1.38
2	D	159	HIS	CD2-NE2	-5.88	1.31	1.37
2	B	106	HIS	CD2-NE2	-5.80	1.31	1.37
2	B	26	HIS	CD2-NE2	-5.76	1.31	1.37
1	C	183	HIS	CD2-NE2	-5.70	1.31	1.37
1	E	183	HIS	CD2-NE2	-5.63	1.31	1.37
2	F	142	HIS	CD2-NE2	-5.57	1.31	1.37
1	C	18	HIS	CD2-NE2	-5.52	1.31	1.37
2	B	64	HIS	CG-ND1	-5.49	1.32	1.38
1	A	183	HIS	CD2-NE2	-5.47	1.31	1.37
2	B	142	HIS	CD2-NE2	-5.42	1.31	1.37
1	C	184	HIS	CG-ND1	-5.41	1.32	1.38
2	F	106	HIS	CG-ND1	-5.39	1.32	1.38
1	E	183	HIS	CG-ND1	-5.38	1.32	1.38
2	D	64	HIS	CD2-NE2	-5.36	1.31	1.37
2	B	142	HIS	CG-ND1	-5.33	1.32	1.38
2	B	64	HIS	CD2-NE2	-5.32	1.31	1.37
1	E	56	HIS	CG-ND1	-5.30	1.32	1.38
1	A	184	HIS	CG-ND1	-5.20	1.32	1.38
2	D	142	HIS	CG-ND1	-5.19	1.32	1.38
1	E	75	HIS	CG-ND1	-5.14	1.32	1.38
2	F	142	HIS	CG-ND1	-5.12	1.32	1.38
1	A	75	HIS	CG-ND1	-5.09	1.32	1.38
1	E	305	CYS	CA-CB	-5.03	1.47	1.54
2	F	26	HIS	CG-ND1	-5.03	1.32	1.38

All (201) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	79	ASP	CA-CB-CG	9.40	122.00	112.60
2	D	28	ASN	CB-CG-ND2	9.35	130.42	116.40
2	F	79	ASP	CA-CB-CG	9.22	121.82	112.60
2	D	79	ASP	CA-CB-CG	9.19	121.79	112.60
2	F	172	GLN	OE1-CD-NE2	-9.02	113.58	122.60
2	D	28	ASN	OD1-CG-ND2	-8.72	113.88	122.60
2	B	160	ASP	CA-CB-CG	-8.63	103.97	112.60
2	F	160	ASP	CA-CB-CG	-8.39	104.21	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	184	HIS	ND1-CG-CD2	8.37	114.47	106.10
2	D	160	ASP	CA-CB-CG	-8.37	104.23	112.60
2	F	9	PHE	CA-CB-CG	8.31	122.11	113.80
2	D	9	PHE	CA-CB-CG	8.23	122.03	113.80
1	C	156	LYS	N-CA-C	8.23	120.53	110.41
1	A	184	HIS	ND1-CG-CD2	8.17	114.27	106.10
1	E	184	HIS	ND1-CG-CD2	7.97	114.07	106.10
1	E	152	ASN	OD1-CG-ND2	-7.96	114.64	122.60
2	B	159	HIS	ND1-CG-CD2	7.93	114.03	106.10
2	F	127	ARG	CA-CB-CG	-7.91	98.28	114.10
2	B	9	PHE	CA-CB-CG	7.90	121.70	113.80
2	D	135	ASN	OD1-CG-ND2	-7.89	114.70	122.60
2	D	127	ARG	CA-CB-CG	-7.87	98.37	114.10
1	E	56	HIS	ND1-CG-CD2	7.86	113.96	106.10
2	B	127	ARG	CA-CB-CG	-7.83	98.44	114.10
1	C	56	HIS	ND1-CG-CD2	7.82	113.92	106.10
2	B	58	LYS	N-CA-C	7.62	121.57	111.28
2	F	58	LYS	N-CA-C	7.58	121.52	111.28
2	B	106	HIS	ND1-CG-CD2	7.52	113.62	106.10
2	B	27	GLN	N-CA-C	-7.52	96.98	109.24
2	F	106	HIS	ND1-CG-CD2	7.49	113.58	106.10
1	E	309	VAL	N-CA-CB	-7.42	98.62	112.36
2	F	60	ASN	OD1-CG-ND2	-7.42	115.18	122.60
2	D	58	LYS	N-CA-C	7.38	121.24	111.28
1	A	152	ASN	OD1-CG-ND2	-7.22	115.38	122.60
1	C	309	VAL	N-CA-CB	-7.21	99.02	112.36
1	C	8	ASN	CA-CB-CG	7.10	119.70	112.60
2	B	60	ASN	OD1-CG-ND2	-7.10	115.50	122.60
2	D	106	HIS	ND1-CG-CD2	7.08	113.18	106.10
1	E	28	THR	CA-CB-OG1	-7.05	99.03	109.60
2	B	169	ASN	CA-CB-CG	7.02	119.62	112.60
2	F	75	GLY	O-C-N	-6.97	118.55	123.08
2	D	159	HIS	ND1-CG-CD2	6.97	113.07	106.10
1	A	85	ASP	N-CA-C	-6.96	104.43	113.12
2	F	159	HIS	ND1-CG-CD2	6.95	113.05	106.10
2	D	60	ASN	OD1-CG-ND2	-6.92	115.67	122.60
1	A	56	HIS	ND1-CG-CD2	6.92	113.02	106.10
2	D	172	GLN	CA-CB-CG	6.92	127.93	114.10
2	D	57	GLU	CA-CB-CG	6.87	127.84	114.10
2	F	27	GLN	OE1-CD-NE2	-6.86	115.75	122.60
2	B	57	GLU	CA-CB-CG	6.85	127.79	114.10
2	F	57	GLU	CA-CB-CG	6.83	127.75	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	28	THR	N-CA-CB	-6.74	100.56	111.22
1	A	28	THR	CA-CB-OG1	-6.74	99.49	109.60
1	C	152	ASN	OD1-CG-ND2	-6.73	115.87	122.60
1	A	8	ASN	CA-CB-CG	6.73	119.33	112.60
1	A	28	THR	N-CA-CB	-6.71	100.62	111.22
1	A	291	ASP	CA-CB-CG	6.66	119.26	112.60
2	F	172	GLN	CG-CD-NE2	6.64	126.36	116.40
1	A	309	VAL	N-CA-CB	-6.61	100.14	112.36
1	A	83	THR	CA-CB-OG1	-6.60	99.69	109.60
2	F	169	ASN	CA-CB-CG	6.54	119.14	112.60
2	D	169	ASN	CA-CB-CG	6.41	119.01	112.60
1	C	85	ASP	N-CA-C	-6.40	105.12	113.12
1	C	56	HIS	CB-CG-CD2	-6.32	122.98	131.20
1	C	6	ASN	OD1-CG-ND2	-6.31	116.29	122.60
2	B	31	GLY	N-CA-C	6.29	119.97	111.72
1	C	252	ILE	N-CA-C	-6.24	97.99	106.85
1	E	85	ASP	N-CA-C	-6.23	105.34	113.12
1	E	75	HIS	CA-CB-CG	6.22	120.03	113.80
1	C	28	THR	CA-CB-OG1	-6.20	100.31	109.60
1	E	103	PRO	N-CA-C	-6.18	101.51	111.03
1	C	255	ARG	NE-CZ-NH1	-6.18	115.32	121.50
1	E	252	ILE	N-CA-C	-6.17	98.08	106.85
1	E	309	VAL	CB-CA-C	6.17	120.73	110.30
1	C	291	ASP	CA-CB-CG	6.17	118.77	112.60
1	E	291	ASP	CA-CB-CG	6.16	118.76	112.60
1	A	78	VAL	CB-CA-C	-6.15	103.98	112.04
1	E	104	ASP	CA-C-O	6.13	128.83	121.65
1	C	28	THR	N-CA-CB	-6.08	101.15	111.31
1	C	183	HIS	ND1-CG-CD2	6.08	112.18	106.10
2	B	92	TRP	CG-CD2-CE3	6.06	139.96	133.90
1	E	26	VAL	N-CA-CB	-6.02	101.23	112.36
1	C	83	THR	CA-CB-OG1	-6.02	100.58	109.60
1	A	323	VAL	CA-C-N	6.01	125.97	119.78
1	A	323	VAL	C-N-CA	6.01	125.97	119.78
1	C	103	PRO	N-CA-C	-6.01	101.77	111.03
1	C	309	VAL	CB-CA-C	6.00	120.44	110.30
1	C	184	HIS	CG-CD2-NE2	-5.99	101.21	107.20
1	E	37	THR	CA-CB-OG1	-5.98	100.63	109.60
1	E	28	THR	CA-CB-CG2	5.96	120.64	110.50
1	C	75	HIS	CA-CB-CG	5.94	119.74	113.80
1	E	152	ASN	CB-CG-ND2	5.92	125.28	116.40
1	E	183	HIS	ND1-CG-CD2	5.91	112.01	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	170	ARG	NE-CZ-NH1	-5.88	115.62	121.50
2	B	25	ARG	NE-CZ-NH1	-5.87	115.63	121.50
1	C	26	VAL	N-CA-CB	-5.87	101.50	112.36
2	B	60	ASN	CA-CB-CG	5.86	118.45	112.60
1	C	28	THR	CA-CB-CG2	5.83	120.40	110.50
1	C	37	THR	CA-CB-OG1	-5.80	100.90	109.60
1	A	75	HIS	CA-CB-CG	5.78	119.58	113.80
1	A	103	PRO	N-CA-C	-5.78	102.13	111.03
1	A	152	ASN	CB-CG-ND2	5.77	125.06	116.40
1	A	184	HIS	CG-CD2-NE2	-5.77	101.43	107.20
2	B	10	ILE	N-CA-CB	-5.77	106.47	112.06
1	A	28	THR	CA-CB-CG2	5.76	120.30	110.50
1	A	58	ILE	N-CA-CB	-5.76	104.47	111.21
1	A	255	ARG	NE-CZ-NH1	-5.76	115.74	121.50
1	A	56	HIS	CB-CG-CD2	-5.76	123.72	131.20
1	A	161	TYR	CA-C-N	5.75	126.21	120.52
1	A	161	TYR	C-N-CA	5.75	126.21	120.52
1	A	83	THR	N-CA-CB	-5.75	100.72	111.13
1	C	321	ARG	NE-CZ-NH1	-5.75	115.75	121.50
1	A	309	VAL	CB-CA-C	5.74	120.00	110.30
1	C	8	ASN	OD1-CG-ND2	-5.74	116.86	122.60
1	E	83	THR	CA-CB-OG1	-5.73	101.01	109.60
1	E	184	HIS	CG-CD2-NE2	-5.72	101.48	107.20
2	D	10	ILE	N-CA-CB	-5.72	106.51	112.06
2	F	27	GLN	CG-CD-NE2	5.69	124.93	116.40
1	E	56	HIS	CB-CG-CD2	-5.68	123.82	131.20
1	E	83	THR	N-CA-CB	-5.68	100.85	111.13
1	C	152	ASN	CB-CG-ND2	5.65	124.87	116.40
1	E	255	ARG	NE-CZ-NH1	-5.64	115.86	121.50
1	E	323	VAL	CA-C-N	5.62	125.93	119.92
1	E	323	VAL	C-N-CA	5.62	125.93	119.92
2	F	133	MET	CB-CG-SD	-5.58	95.97	112.70
1	A	104	ASP	CA-C-O	5.57	128.17	121.65
2	D	92	TRP	CG-CD2-CE3	5.56	139.46	133.90
1	C	323	VAL	CA-C-N	5.55	125.86	119.92
1	C	323	VAL	C-N-CA	5.55	125.86	119.92
1	C	104	ASP	CA-C-O	5.55	128.14	121.65
1	A	26	VAL	N-CA-CB	-5.54	102.12	112.36
1	E	272	ALA	CA-C-N	5.54	125.46	119.76
1	E	272	ALA	C-N-CA	5.54	125.46	119.76
1	A	37	THR	CA-CB-OG1	-5.53	101.30	109.60
1	A	252	ILE	N-CA-C	-5.48	99.06	106.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	76	ARG	N-CA-C	5.48	117.69	111.11
2	F	27	GLN	N-CA-C	-5.48	99.36	108.34
1	C	272	ALA	CA-C-N	5.47	125.39	119.76
1	C	272	ALA	C-N-CA	5.47	125.39	119.76
1	A	321	ARG	NE-CZ-NH1	-5.46	116.04	121.50
2	F	60	ASN	CA-CB-CG	5.46	118.06	112.60
1	E	184	HIS	CB-CG-CD2	-5.44	124.12	131.20
1	E	170	ASN	CA-CB-CG	-5.44	107.16	112.60
1	C	184	HIS	CB-CG-CD2	-5.44	124.13	131.20
1	E	298	ASN	OD1-CG-ND2	-5.44	117.16	122.60
2	B	159	HIS	CG-CD2-NE2	-5.41	101.79	107.20
2	F	14	TRP	CG-CD2-CE3	5.38	139.28	133.90
1	C	133	ASN	CA-CB-CG	-5.37	107.23	112.60
1	A	272	ALA	CA-C-N	5.37	125.29	119.76
1	A	272	ALA	C-N-CA	5.37	125.29	119.76
1	C	321	ARG	CB-CG-CD	-5.36	98.97	111.30
2	D	14	TRP	CG-CD2-CE3	5.36	139.26	133.90
2	F	10	ILE	N-CA-CB	-5.36	106.86	112.06
2	D	64	HIS	CB-CG-CD2	-5.34	124.25	131.20
1	C	170	ASN	CA-CB-CG	-5.34	107.26	112.60
2	F	92	TRP	CG-CD2-CE3	5.32	139.22	133.90
2	B	14	TRP	CG-CD2-CE3	5.32	139.22	133.90
2	F	95	ASN	OD1-CG-ND2	-5.31	117.29	122.60
1	A	184	HIS	CB-CG-CD2	-5.27	124.35	131.20
1	C	73	ASP	CA-C-N	5.27	124.72	119.24
1	C	73	ASP	C-N-CA	5.27	124.72	119.24
1	A	22	ASN	CA-C-O	-5.26	112.98	120.51
1	A	110	SER	N-CA-CB	5.26	117.59	109.91
1	C	78	VAL	CB-CA-C	-5.26	105.15	112.04
1	C	83	THR	N-CA-CB	-5.26	101.61	111.13
1	E	73	ASP	CA-C-N	5.26	124.71	119.24
1	E	73	ASP	C-N-CA	5.26	124.71	119.24
1	A	133	ASN	CA-CB-CG	-5.22	107.38	112.60
1	A	180	TRP	CE2-CD2-CG	-5.22	100.94	107.20
1	A	253	ALA	N-CA-C	5.22	117.86	110.24
1	E	101	ASP	CA-CB-CG	5.21	117.81	112.60
1	C	327	GLN	CA-CB-CG	5.21	124.52	114.10
1	A	321	ARG	CB-CG-CD	-5.20	99.33	111.30
1	A	183	HIS	ND1-CG-CD2	5.20	111.30	106.10
2	B	28	ASN	CA-CB-CG	5.20	117.80	112.60
1	E	253	ALA	N-CA-C	5.19	117.82	110.24
2	B	95	ASN	OD1-CG-ND2	-5.18	117.42	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	253	ALA	N-CA-C	5.17	117.79	110.24
2	B	172	GLN	OE1-CD-NE2	-5.17	117.43	122.60
1	A	73	ASP	CA-C-N	5.16	124.60	119.24
1	A	73	ASP	C-N-CA	5.16	124.60	119.24
1	E	286	GLY	N-CA-C	-5.15	105.67	111.85
2	D	60	ASN	CA-CB-CG	5.15	117.75	112.60
1	A	156	LYS	CA-C-N	-5.13	115.01	122.65
1	A	156	LYS	C-N-CA	-5.13	115.01	122.65
1	C	180	TRP	CE2-CD2-CG	-5.13	101.05	107.20
1	E	37	THR	CA-CB-CG2	5.10	119.17	110.50
1	E	133	ASN	CA-CB-CG	-5.10	107.50	112.60
1	E	78	VAL	CB-CA-C	-5.09	105.38	112.04
2	B	106	HIS	CG-CD2-NE2	-5.08	102.12	107.20
1	E	189	GLN	CA-CB-CG	5.07	124.25	114.10
1	C	296	ASN	N-CA-CB	-5.06	103.08	111.49
2	D	170	ARG	NE-CZ-NH1	-5.06	116.44	121.50
1	C	325	GLU	CB-CG-CD	5.05	121.19	112.60
2	D	49	ASN	OD1-CG-ND2	-5.04	117.56	122.60
2	D	95	ASN	OD1-CG-ND2	-5.03	117.57	122.60
1	E	22	ASN	CA-C-O	-5.02	113.33	120.51
1	E	180	TRP	CG-CD2-CE3	5.02	138.92	133.90
2	F	106	HIS	CG-CD2-NE2	-5.02	102.18	107.20
1	E	110	SER	CB-CA-C	-5.01	103.24	110.96
1	A	210	GLN	OE1-CD-NE2	-5.01	117.59	122.60
1	E	321	ARG	CB-CG-CD	-5.01	99.78	111.30

There are no chirality outliers.

There are no planarity outliers.

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	2532	0	2473	40	0
1	C	2532	0	2473	39	0
1	E	2532	0	2473	38	0
2	B	1417	0	1344	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1417	0	1344	28	0
2	F	1417	0	1344	26	0
3	G	39	0	34	0	0
3	H	39	0	34	0	0
3	I	39	0	34	0	0
4	A	21	0	18	1	0
4	C	21	0	18	1	0
4	E	21	0	18	1	0
5	A	42	0	39	0	0
5	B	14	0	13	0	0
5	C	42	0	39	0	0
5	D	14	0	13	0	0
5	E	42	0	39	0	0
5	F	14	0	13	0	0
6	A	8	0	0	0	0
6	B	5	0	0	0	0
6	C	8	0	0	0	0
6	D	5	0	0	0	0
6	E	9	0	0	0	0
6	F	4	0	0	0	0
All	All	12234	0	11763	163	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (163) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:HIS:HD2	2:B:28:ASN:HB3	1.47	0.78
2:B:133:MET:HE3	2:B:139:LYS:HB2	1.69	0.73
1:A:10:THR:HG22	2:B:141:TYR:HA	1.70	0.73
1:E:10:THR:HG22	2:F:141:TYR:HA	1.70	0.73
2:B:132:GLU:HG2	2:B:134:GLY:H	1.53	0.72
2:D:132:GLU:HG2	2:D:134:GLY:H	1.55	0.72
2:F:132:GLU:HG2	2:F:134:GLY:H	1.54	0.71
1:C:10:THR:HG22	2:D:141:TYR:HA	1.74	0.69
2:D:28:ASN:HB2	2:D:144:CYS:O	1.93	0.68
1:C:155:THR:HG21	4:C:329:SIA:H111	1.76	0.68
1:A:155:THR:HG21	4:A:329:SIA:H111	1.76	0.66
1:C:29:ILE:HD11	2:D:102:LEU:HD12	1.77	0.66
1:E:155:THR:HG21	4:E:329:SIA:H111	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:29:ILE:HD11	2:F:102:LEU:HD12	1.78	0.66
1:C:77:ASP:O	1:C:80:GLN:HG3	1.97	0.64
1:C:216:ASN:HB3	1:E:212:THR:HG21	1.80	0.62
1:A:29:ILE:HD11	2:B:102:LEU:HD12	1.80	0.62
1:A:77:ASP:O	1:A:80:GLN:HG3	2.00	0.61
1:C:283:THR:HG22	1:C:301:THR:HG22	1.85	0.58
1:E:77:ASP:O	1:E:80:GLN:HG3	2.02	0.58
2:B:141:TYR:O	2:B:166:ALA:HA	2.03	0.58
2:D:141:TYR:O	2:D:166:ALA:HA	2.03	0.58
1:A:283:THR:HG22	1:A:301:THR:HG22	1.86	0.57
1:E:180:TRP:HH2	1:E:213:ILE:HD13	1.69	0.57
1:E:283:THR:HG22	1:E:301:THR:HG22	1.87	0.56
2:D:6:ILE:HD12	2:D:112:GLY:HA2	1.87	0.56
1:C:180:TRP:HH2	1:C:213:ILE:HD13	1.70	0.56
1:E:175:ASP:OD1	1:E:239:PRO:HD3	2.06	0.56
1:C:67:ILE:HD12	1:C:108:LEU:HD13	1.87	0.56
2:B:6:ILE:HD12	2:B:112:GLY:HA2	1.88	0.55
1:A:180:TRP:HH2	1:A:213:ILE:HD13	1.71	0.55
2:D:126:LEU:HD21	2:D:152:ILE:HD13	1.87	0.55
2:F:141:TYR:O	2:F:166:ALA:HA	2.07	0.55
2:F:126:LEU:HD21	2:F:152:ILE:HD13	1.88	0.54
2:B:126:LEU:HD21	2:B:152:ILE:HD13	1.90	0.54
1:C:175:ASP:OD1	1:C:239:PRO:HD3	2.07	0.53
1:A:175:ASP:OD1	1:A:239:PRO:HD3	2.09	0.53
1:A:67:ILE:HD12	1:A:108:LEU:HD13	1.91	0.53
1:E:67:ILE:HD12	1:E:108:LEU:HD13	1.90	0.52
2:F:6:ILE:HD12	2:F:112:GLY:HA2	1.91	0.51
1:C:183:HIS:HA	1:C:230:ILE:HG22	1.93	0.51
1:E:311:GLN:HE21	2:F:97:GLU:HB2	1.75	0.50
1:E:183:HIS:HA	1:E:230:ILE:HG22	1.94	0.50
1:E:102:VAL:HG22	1:E:232:ILE:HB	1.94	0.49
1:E:56:HIS:ND1	1:E:264:LYS:NZ	2.60	0.49
1:A:311:GLN:HE21	2:B:97:GLU:HB2	1.78	0.49
1:A:183:HIS:HA	1:A:230:ILE:HG22	1.96	0.48
1:C:102:VAL:HG22	1:C:232:ILE:HB	1.95	0.48
1:E:222:TRP:CE2	1:E:225:GLY:HA2	2.49	0.48
1:E:311:GLN:NE2	2:F:97:GLU:HB2	2.28	0.48
1:A:21:PRO:HB2	1:A:328:THR:HA	1.95	0.48
1:A:56:HIS:ND1	1:A:264:LYS:NZ	2.62	0.48
1:C:311:GLN:NE2	2:D:97:GLU:HB2	2.29	0.48
1:C:311:GLN:HE21	2:D:97:GLU:HB2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:HIS:ND1	1:C:264:LYS:NZ	2.61	0.47
1:A:311:GLN:NE2	2:B:97:GLU:HB2	2.29	0.47
1:A:21:PRO:CB	1:A:328:THR:HA	2.45	0.47
1:A:222:TRP:CE2	1:A:225:GLY:HA2	2.49	0.47
2:B:163:ARG:O	2:B:167:LEU:HB2	2.15	0.47
2:B:83:TYR:O	2:B:87:THR:HG23	2.15	0.47
1:C:156:LYS:HB2	1:C:160:THR:O	2.14	0.47
2:D:163:ARG:O	2:D:167:LEU:HB2	2.15	0.47
1:E:54:ASN:O	1:E:278:ILE:HA	2.14	0.47
1:E:180:TRP:CH2	1:E:213:ILE:HD13	2.49	0.47
1:A:102:VAL:HG22	1:A:232:ILE:HB	1.96	0.47
1:A:117:THR:HG21	1:A:261:ARG:HH21	1.80	0.47
2:F:163:ARG:O	2:F:167:LEU:HB2	2.15	0.47
1:C:222:TRP:CE2	1:C:225:GLY:HA2	2.49	0.46
1:C:102:VAL:HG11	1:C:108:LEU:HD12	1.97	0.46
2:D:27:GLN:HG3	2:D:32:THR:HG23	1.97	0.46
1:A:102:VAL:HG11	1:A:108:LEU:HD12	1.97	0.46
2:D:87:THR:HG21	2:F:88:LYS:HD2	1.98	0.46
1:A:54:ASN:O	1:A:278:ILE:HA	2.16	0.46
1:A:133:ASN:H	1:A:152:ASN:ND2	2.13	0.46
1:E:15:LEU:HD23	2:F:118:LEU:HD13	1.97	0.46
1:A:212:THR:HG21	1:E:216:ASN:HB3	1.98	0.46
2:B:26:HIS:CD2	2:B:28:ASN:HB3	2.38	0.46
1:C:54:ASN:O	1:C:278:ILE:HA	2.16	0.46
1:C:117:THR:HG21	1:C:261:ARG:HH21	1.80	0.46
1:A:197:GLN:HG3	1:A:248:ASN:HD22	1.81	0.46
2:B:54:ARG:NH1	1:E:27:LYS:HD3	2.31	0.45
1:C:133:ASN:H	1:C:152:ASN:ND2	2.13	0.45
1:E:102:VAL:HG11	1:E:108:LEU:HD12	1.98	0.45
1:A:15:LEU:HD23	2:B:118:LEU:HD13	1.99	0.45
1:A:180:TRP:CH2	1:A:213:ILE:HD13	2.51	0.45
1:C:66:LEU:HD22	1:C:267:ILE:HD12	1.99	0.45
1:E:17:HIS:CD2	2:F:6:ILE:HG12	2.52	0.45
2:B:91:LEU:HD13	2:F:91:LEU:HD13	1.99	0.45
1:A:66:LEU:HD22	1:A:267:ILE:HD12	1.98	0.45
2:D:2:LEU:HB3	2:F:3:PHE:HZ	1.81	0.45
1:E:52:CYS:HB3	1:E:277:CYS:O	2.17	0.45
1:A:325:GLU:HG3	2:B:13:GLY:O	2.17	0.44
1:C:180:TRP:CH2	1:C:213:ILE:HD13	2.50	0.44
1:C:15:LEU:HD23	2:D:118:LEU:HD13	1.99	0.44
2:D:26:HIS:ND1	2:D:149:ILE:HG21	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:151:SER:HA	2:D:154:ASN:OD1	2.17	0.44
1:A:309:VAL:HG22	2:B:93:SER:HA	2.00	0.44
1:C:14:CYS:HA	2:D:137:CYS:HA	2.00	0.44
1:A:14:CYS:HA	2:B:137:CYS:HA	2.00	0.44
2:B:57:GLU:HG2	2:B:58:LYS:HG3	1.99	0.44
1:E:14:CYS:HA	2:F:137:CYS:HA	2.00	0.44
1:C:27:LYS:HD3	2:F:54:ARG:NH1	2.32	0.44
1:C:52:CYS:HB3	1:C:277:CYS:O	2.18	0.43
1:C:182:ILE:HD11	1:C:215:PRO:HD3	2.00	0.43
2:D:57:GLU:HG2	2:D:58:LYS:HG3	2.00	0.43
1:C:197:GLN:HG3	1:C:248:ASN:HD22	1.83	0.43
1:E:197:GLN:HG3	1:E:248:ASN:HD22	1.82	0.43
1:C:325:GLU:HB2	2:D:12:ASN:ND2	2.33	0.43
2:B:25:ARG:HA	2:B:34:GLN:HA	2.01	0.43
2:D:30:GLU:HG3	2:D:146:ASN:ND2	2.34	0.43
1:E:43:VAL:HG23	1:E:314:LEU:HB2	1.99	0.43
1:E:71:LEU:O	1:E:148:PHE:HB3	2.18	0.43
1:C:43:VAL:HG23	1:C:314:LEU:HB2	2.00	0.43
1:C:228:SER:O	1:C:229:ARG:HD2	2.18	0.43
1:E:133:ASN:H	1:E:152:ASN:ND2	2.15	0.43
1:E:182:ILE:HD11	1:E:215:PRO:HD3	2.01	0.43
1:E:228:SER:O	1:E:229:ARG:HD2	2.19	0.43
2:D:133:MET:HG2	2:D:137:CYS:O	2.18	0.43
1:A:228:SER:O	1:A:229:ARG:HD2	2.19	0.42
2:B:153:ARG:HH21	2:B:153:ARG:HD2	1.70	0.42
2:B:39:LYS:HE2	2:B:39:LYS:HB3	1.85	0.42
1:E:117:THR:HG21	1:E:261:ARG:HH21	1.83	0.42
1:E:309:VAL:HG22	2:F:93:SER:HA	2.01	0.42
1:C:17:HIS:CD2	2:D:6:ILE:HG12	2.54	0.42
2:D:2:LEU:HB3	2:F:3:PHE:CZ	2.54	0.42
1:A:182:ILE:HD11	1:A:215:PRO:HD3	2.02	0.42
2:B:151:SER:HA	2:B:154:ASN:OD1	2.20	0.42
1:C:326:LYS:HD3	1:C:328:THR:O	2.20	0.42
1:A:17:HIS:CD2	2:B:6:ILE:HG12	2.54	0.42
1:A:102:VAL:HB	1:A:105:TYR:HD2	1.85	0.42
1:C:133:ASN:H	1:C:152:ASN:HD21	1.67	0.42
2:F:25:ARG:HG3	2:F:34:GLN:HG3	2.02	0.42
2:B:163:ARG:NH1	2:F:131:GLU:OE2	2.53	0.42
1:A:43:VAL:HG23	1:A:314:LEU:HB2	2.01	0.42
1:E:102:VAL:HB	1:E:105:TYR:HD2	1.85	0.42
2:D:27:GLN:HG3	2:D:32:THR:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ASN:OD1	1:A:276:THR:HA	2.20	0.41
2:F:57:GLU:HG2	2:F:58:LYS:HG3	2.01	0.41
2:F:83:TYR:O	2:F:87:THR:HG23	2.21	0.41
2:D:5:ALA:HA	2:D:9:PHE:CE2	2.55	0.41
1:A:52:CYS:HB3	1:A:277:CYS:O	2.20	0.41
1:C:71:LEU:O	1:C:148:PHE:HB3	2.20	0.41
1:C:309:VAL:HG22	2:D:93:SER:HA	2.03	0.41
1:C:102:VAL:HB	1:C:105:TYR:HD2	1.85	0.41
2:D:39:LYS:HB3	2:D:39:LYS:HE2	1.87	0.41
2:F:5:ALA:HA	2:F:9:PHE:CE2	2.55	0.41
1:A:101:ASP:O	1:A:231:SER:HA	2.21	0.41
2:B:5:ALA:HA	2:B:9:PHE:CE2	2.56	0.41
2:B:127:ARG:NH2	2:F:131:GLU:OE1	2.54	0.41
1:C:53:ASN:OD1	1:C:276:THR:HA	2.21	0.41
2:D:5:ALA:HA	2:D:9:PHE:CD2	2.56	0.41
1:E:66:LEU:HD22	1:E:267:ILE:HD12	2.01	0.41
1:E:53:ASN:OD1	1:E:276:THR:HA	2.22	0.40
1:A:133:ASN:H	1:A:152:ASN:HD21	1.68	0.40
1:A:244:VAL:CG2	1:E:221:PRO:HG3	2.51	0.40
1:C:216:ASN:HB2	1:C:220:ARG:HH12	1.87	0.40
1:A:161:TYR:CE1	1:A:249:GLY:HA2	2.56	0.40
1:E:133:ASN:H	1:E:152:ASN:HD21	1.70	0.40
2:F:151:SER:HA	2:F:154:ASN:OD1	2.22	0.40
1:A:213:ILE:HG12	1:A:233:TYR:CZ	2.56	0.40
2:F:133:MET:HE3	2:F:139:LYS:HB2	2.04	0.40
2:B:5:ALA:HA	2:B:9:PHE:CD2	2.57	0.40
1:E:89:GLU:OE2	1:E:109:ARG:NH2	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	326/328 (99%)	307 (94%)	18 (6%)	1 (0%)	36	68
1	C	326/328 (99%)	311 (95%)	13 (4%)	2 (1%)	21	56
1	E	326/328 (99%)	312 (96%)	12 (4%)	2 (1%)	21	56
2	B	173/175 (99%)	161 (93%)	9 (5%)	3 (2%)	7	35
2	D	173/175 (99%)	162 (94%)	10 (6%)	1 (1%)	21	56
2	F	173/175 (99%)	163 (94%)	9 (5%)	1 (1%)	21	56
All	All	1497/1509 (99%)	1416 (95%)	71 (5%)	10 (1%)	18	52

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	29	SER
2	B	30	GLU
1	C	327	GLN
1	A	62	ILE
1	C	62	ILE
1	E	62	ILE
2	B	127	ARG
2	D	127	ARG
1	E	158	GLY
2	F	127	ARG

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	289/289 (100%)	257 (89%)	32 (11%)	6	25
1	C	289/289 (100%)	259 (90%)	30 (10%)	7	28
1	E	289/289 (100%)	259 (90%)	30 (10%)	7	28
2	B	148/148 (100%)	131 (88%)	17 (12%)	5	24
2	D	148/148 (100%)	132 (89%)	16 (11%)	6	27
2	F	148/148 (100%)	135 (91%)	13 (9%)	9	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1311/1311 (100%)	1173 (90%)	138 (10%)	6 28

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	13	LEU
1	A	18	HIS
1	A	26	VAL
1	A	28	THR
1	A	31	ASP
1	A	37	THR
1	A	55	PRO
1	A	75	HIS
1	A	83	THR
1	A	92	LYS
1	A	95	SER
1	A	108	LEU
1	A	128	THR
1	A	150	ARG
1	A	159	SER
1	A	160	THR
1	A	164	LEU
1	A	172	ASP
1	A	177	LEU
1	A	197	GLN
1	A	205	SER
1	A	251	LEU
1	A	266	SER
1	A	278	ILE
1	A	291	ASP
1	A	309	VAL
1	A	314	LEU
1	A	318	THR
1	A	321	ARG
1	A	325	GLU
1	A	328	THR
2	B	28	ASN
2	B	29	SER
2	B	38	LEU
2	B	45	ILE
2	B	54	ARG

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Mol	Chain	Res	Type
2	B	56	ILE
2	B	57	GLU
2	B	100	VAL
2	B	110	LEU
2	B	118	LEU
2	B	127	ARG
2	B	128	GLU
2	B	150	GLU
2	B	160	ASP
2	B	172	GLN
2	B	173	ILE
2	B	174	LYS
1	C	13	LEU
1	C	18	HIS
1	C	26	VAL
1	C	28	THR
1	C	31	ASP
1	C	37	THR
1	C	55	PRO
1	C	75	HIS
1	C	83	THR
1	C	92	LYS
1	C	95	SER
1	C	108	LEU
1	C	128	THR
1	C	150	ARG
1	C	156	LYS
1	C	160	THR
1	C	164	LEU
1	C	172	ASP
1	C	177	LEU
1	C	197	GLN
1	C	205	SER
1	C	251	LEU
1	C	266	SER
1	C	278	ILE
1	C	291	ASP
1	C	309	VAL
1	C	314	LEU
1	C	318	THR
1	C	321	ARG
1	C	327	GLN

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Mol	Chain	Res	Type
2	D	28	ASN
2	D	38	LEU
2	D	45	ILE
2	D	54	ARG
2	D	56	ILE
2	D	57	GLU
2	D	100	VAL
2	D	110	LEU
2	D	118	LEU
2	D	127	ARG
2	D	128	GLU
2	D	133	MET
2	D	150	GLU
2	D	160	ASP
2	D	173	ILE
2	D	174	LYS
1	E	13	LEU
1	E	18	HIS
1	E	26	VAL
1	E	28	THR
1	E	37	THR
1	E	55	PRO
1	E	75	HIS
1	E	83	THR
1	E	92	LYS
1	E	95	SER
1	E	108	LEU
1	E	128	THR
1	E	149	SER
1	E	150	ARG
1	E	160	THR
1	E	164	LEU
1	E	172	ASP
1	E	177	LEU
1	E	197	GLN
1	E	205	SER
1	E	251	LEU
1	E	266	SER
1	E	278	ILE
1	E	291	ASP
1	E	309	VAL
1	E	314	LEU

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Mol	Chain	Res	Type
1	E	318	THR
1	E	321	ARG
1	E	327	GLN
1	E	328	THR
2	F	29	SER
2	F	38	LEU
2	F	45	ILE
2	F	54	ARG
2	F	56	ILE
2	F	57	GLU
2	F	110	LEU
2	F	118	LEU
2	F	127	ARG
2	F	128	GLU
2	F	160	ASP
2	F	173	ILE
2	F	174	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	171	ASN
1	A	210	GLN
1	A	248	ASN
2	B	27	GLN
2	B	28	ASN
2	B	49	ASN
2	B	53	ASN
1	C	152	ASN
1	C	171	ASN
1	C	210	GLN
1	C	248	ASN
1	C	327	GLN
2	D	49	ASN
2	D	53	ASN
1	E	1	GLN
1	E	8	ASN
1	E	152	ASN
1	E	171	ASN
1	E	189	GLN
1	E	248	ASN

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Mol	Chain	Res	Type
1	E	327	GLN
2	F	49	ASN
2	F	53	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

9 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	G	1	3,1	14,14,15	0.75	1 (7%)	17,19,21	0.78	0
3	NAG	G	2	3	14,14,15	0.43	0	17,19,21	0.91	1 (5%)
3	MAN	G	3	3	11,11,12	0.84	0	15,15,17	1.22	2 (13%)
3	NAG	H	1	3,1	14,14,15	0.84	1 (7%)	17,19,21	0.88	1 (5%)
3	NAG	H	2	3	14,14,15	0.47	0	17,19,21	0.91	1 (5%)
3	MAN	H	3	3	11,11,12	0.67	0	15,15,17	1.33	2 (13%)
3	NAG	I	1	3,1	14,14,15	0.60	0	17,19,21	0.84	1 (5%)
3	NAG	I	2	3	14,14,15	0.48	0	17,19,21	0.94	1 (5%)
3	MAN	I	3	3	11,11,12	0.75	0	15,15,17	1.23	1 (6%)

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	-	0/6/23/26	0/1/1/1
3	MAN	G	3	3	1/1/4/5	0/2/19/22	0/1/1/1
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	MAN	H	3	3	1/1/4/5	0/2/19/22	0/1/1/1
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	MAN	I	3	3	1/1/4/5	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1	NAG	O5-C1	-2.41	1.39	1.43
3	G	1	NAG	O5-C1	-2.01	1.40	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	3	MAN	C1-O5-C5	3.45	116.81	112.19
3	I	3	MAN	O2-C2-C1	2.60	115.18	109.22
3	H	2	NAG	C4-C3-C2	-2.53	107.31	111.02
3	H	3	MAN	O3-C3-C2	2.53	115.22	110.05
3	I	2	NAG	C4-C3-C2	-2.46	107.42	111.02
3	G	2	NAG	C4-C3-C2	-2.30	107.65	111.02
3	G	3	MAN	C1-C2-C3	-2.28	106.33	109.64
3	G	3	MAN	C3-C4-C5	2.27	114.34	110.23
3	I	1	NAG	C1-O5-C5	2.21	115.14	112.19
3	H	1	NAG	C1-O5-C5	2.11	115.01	112.19

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	3	MAN	C1
3	H	3	MAN	C1
3	I	3	MAN	C1

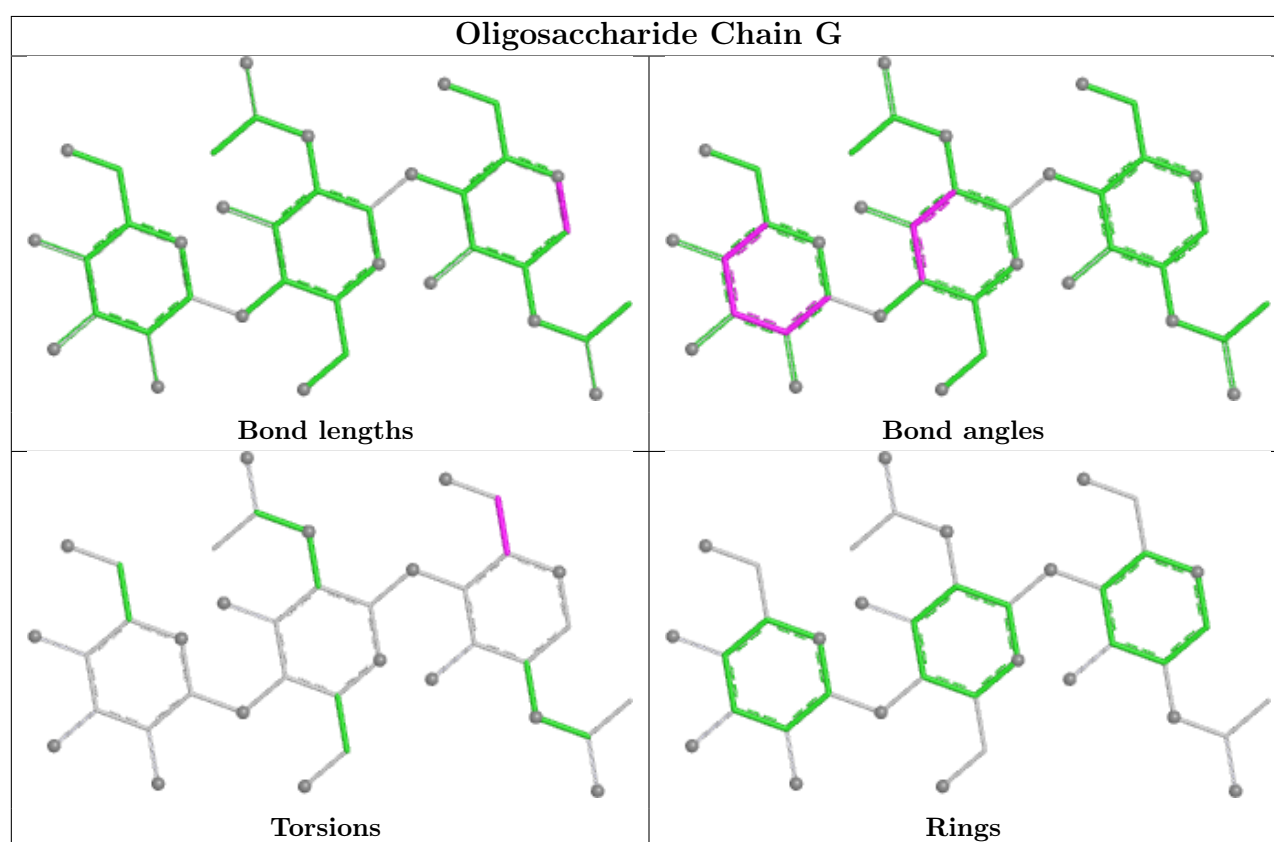
All (6) torsion outliers are listed below:

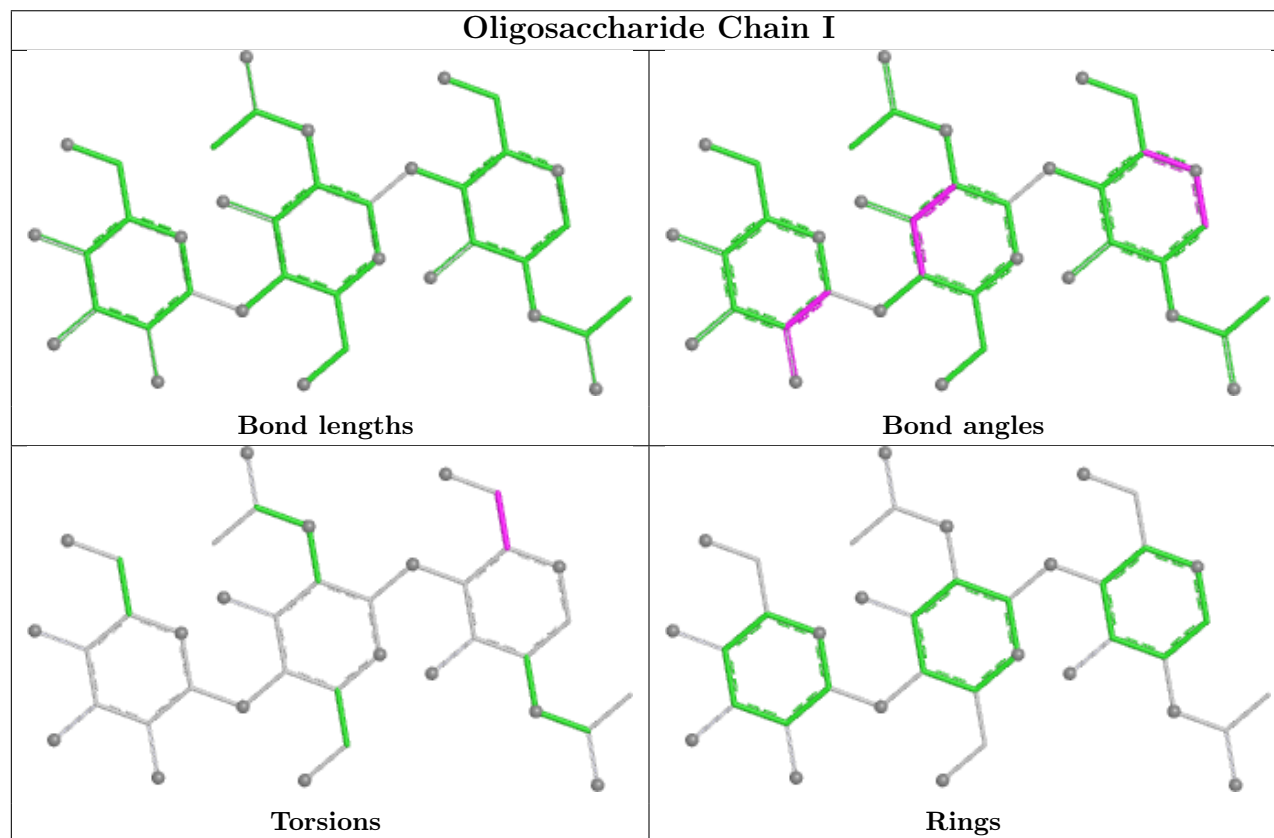
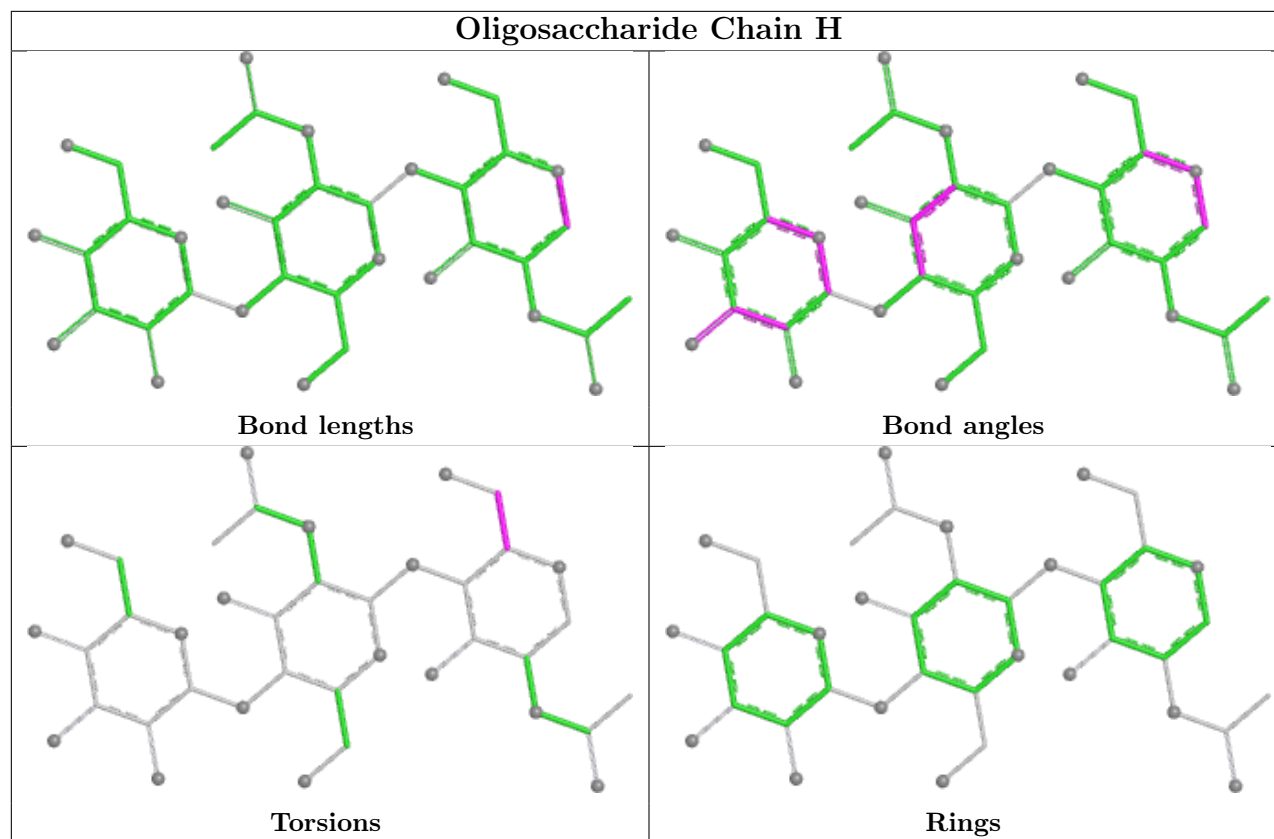
Mol	Chain	Res	Type	Atoms
3	G	1	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6

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

15 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	A	348	1	14,14,15	0.84	1 (7%)	17,19,21	1.08	0
5	NAG	D	401	2	14,14,15	0.73	0	17,19,21	1.19	1 (5%)
4	SIA	C	329	-	21,21,21	1.13	2 (9%)	24,31,31	1.39	3 (12%)
5	NAG	E	334	1	14,14,15	0.92	0	17,19,21	1.42	2 (11%)
5	NAG	E	348	1	14,14,15	0.67	0	17,19,21	1.10	1 (5%)
5	NAG	F	401	2	14,14,15	0.70	0	17,19,21	1.13	1 (5%)
4	SIA	E	329	-	21,21,21	1.10	1 (4%)	24,31,31	1.26	1 (4%)
5	NAG	B	401	2	14,14,15	0.64	0	17,19,21	1.14	1 (5%)
5	NAG	C	334	1	14,14,15	0.91	0	17,19,21	1.38	1 (5%)
5	NAG	C	330	1	14,14,15	0.74	0	17,19,21	1.15	1 (5%)
5	NAG	A	334	1	14,14,15	0.93	0	17,19,21	1.46	2 (11%)
5	NAG	E	330	1	14,14,15	0.90	1 (7%)	17,19,21	1.02	0
5	NAG	C	348	1	14,14,15	0.72	0	17,19,21	1.05	1 (5%)
4	SIA	A	329	-	21,21,21	1.15	2 (9%)	24,31,31	1.30	2 (8%)
5	NAG	A	330	1	14,14,15	0.81	0	17,19,21	1.05	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	348	1	-	1/6/23/26	0/1/1/1
5	NAG	D	401	2	-	0/6/23/26	0/1/1/1
4	SIA	C	329	-	-	0/20/38/38	0/1/1/1
5	NAG	E	334	1	-	1/6/23/26	0/1/1/1
5	NAG	E	348	1	-	1/6/23/26	0/1/1/1
5	NAG	F	401	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SIA	E	329	-	-	1/20/38/38	0/1/1/1
5	NAG	B	401	2	-	0/6/23/26	0/1/1/1
5	NAG	C	334	1	-	1/6/23/26	0/1/1/1
5	NAG	C	330	1	-	0/6/23/26	0/1/1/1
5	NAG	A	334	1	-	1/6/23/26	0/1/1/1
5	NAG	E	330	1	-	1/6/23/26	0/1/1/1
5	NAG	C	348	1	-	1/6/23/26	0/1/1/1
4	SIA	A	329	-	-	0/20/38/38	0/1/1/1
5	NAG	A	330	1	-	2/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	329	SIA	C3-C2	3.94	1.57	1.51
4	C	329	SIA	C3-C2	3.92	1.57	1.51
4	A	329	SIA	C3-C2	3.85	1.56	1.51
5	E	330	NAG	C4-C5	2.49	1.58	1.53
5	A	348	NAG	C1-C2	2.38	1.55	1.52
4	A	329	SIA	O1B-C1	-2.15	1.22	1.30
4	C	329	SIA	O1B-C1	-2.08	1.23	1.30

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	334	NAG	C1-O5-C5	3.53	116.91	112.19
5	E	334	NAG	C1-O5-C5	3.37	116.71	112.19
5	D	401	NAG	C1-O5-C5	3.32	116.63	112.19
5	B	401	NAG	C1-O5-C5	3.16	116.42	112.19
5	C	334	NAG	C1-O5-C5	3.15	116.40	112.19
5	F	401	NAG	C1-O5-C5	2.94	116.12	112.19
4	C	329	SIA	O8-C8-C7	2.47	115.03	109.25
4	C	329	SIA	C8-C7-C6	-2.43	108.48	113.05
4	C	329	SIA	C11-C10-N5	2.36	120.04	116.12
4	A	329	SIA	C8-C7-C6	-2.29	108.75	113.05
5	A	334	NAG	C1-C2-N2	2.21	113.92	110.43
4	E	329	SIA	C8-C7-C6	-2.20	108.91	113.05
5	C	330	NAG	C8-C7-N2	2.17	119.71	116.12
4	A	329	SIA	C11-C10-N5	2.11	119.61	116.12
5	C	348	NAG	C8-C7-N2	2.09	119.58	116.12
5	E	348	NAG	C8-C7-N2	2.06	119.54	116.12
5	E	334	NAG	C8-C7-N2	2.03	119.48	116.12

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	334	NAG	O5-C5-C6-O6
5	C	334	NAG	O5-C5-C6-O6
5	A	334	NAG	O5-C5-C6-O6
5	C	348	NAG	O5-C5-C6-O6
5	A	348	NAG	O5-C5-C6-O6
5	E	348	NAG	O5-C5-C6-O6
5	A	330	NAG	C4-C5-C6-O6
5	A	330	NAG	O5-C5-C6-O6
4	E	329	SIA	O1A-C1-C2-C3
5	E	330	NAG	C4-C5-C6-O6

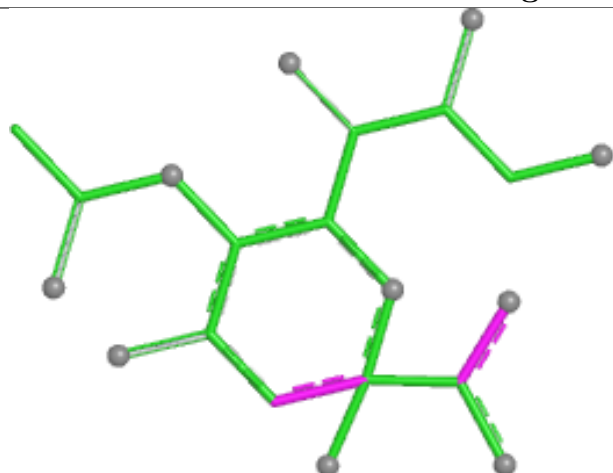
There are no ring outliers.

3 monomers are involved in 3 short contacts:

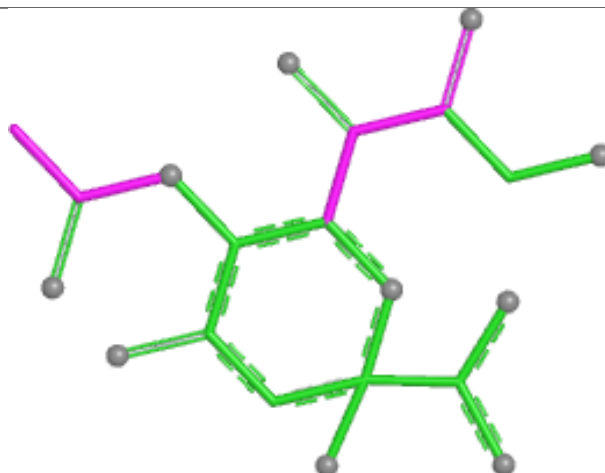
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	329	SIA	1	0
4	E	329	SIA	1	0
4	A	329	SIA	1	0

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

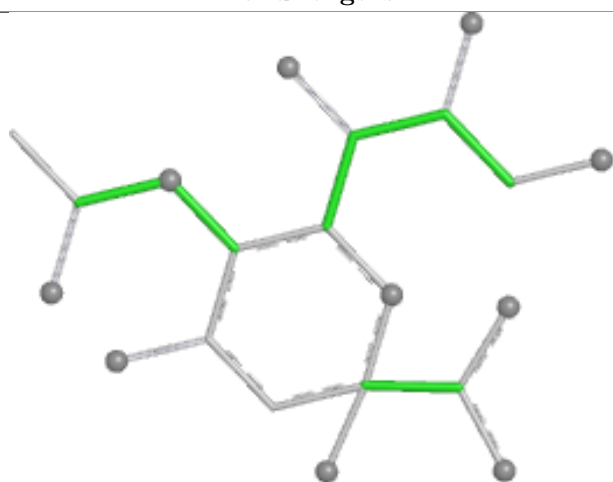
Ligand SIA C 329



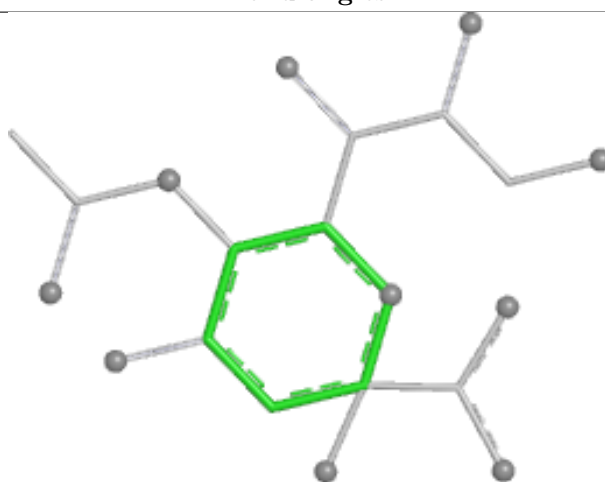
Bond lengths



Bond angles

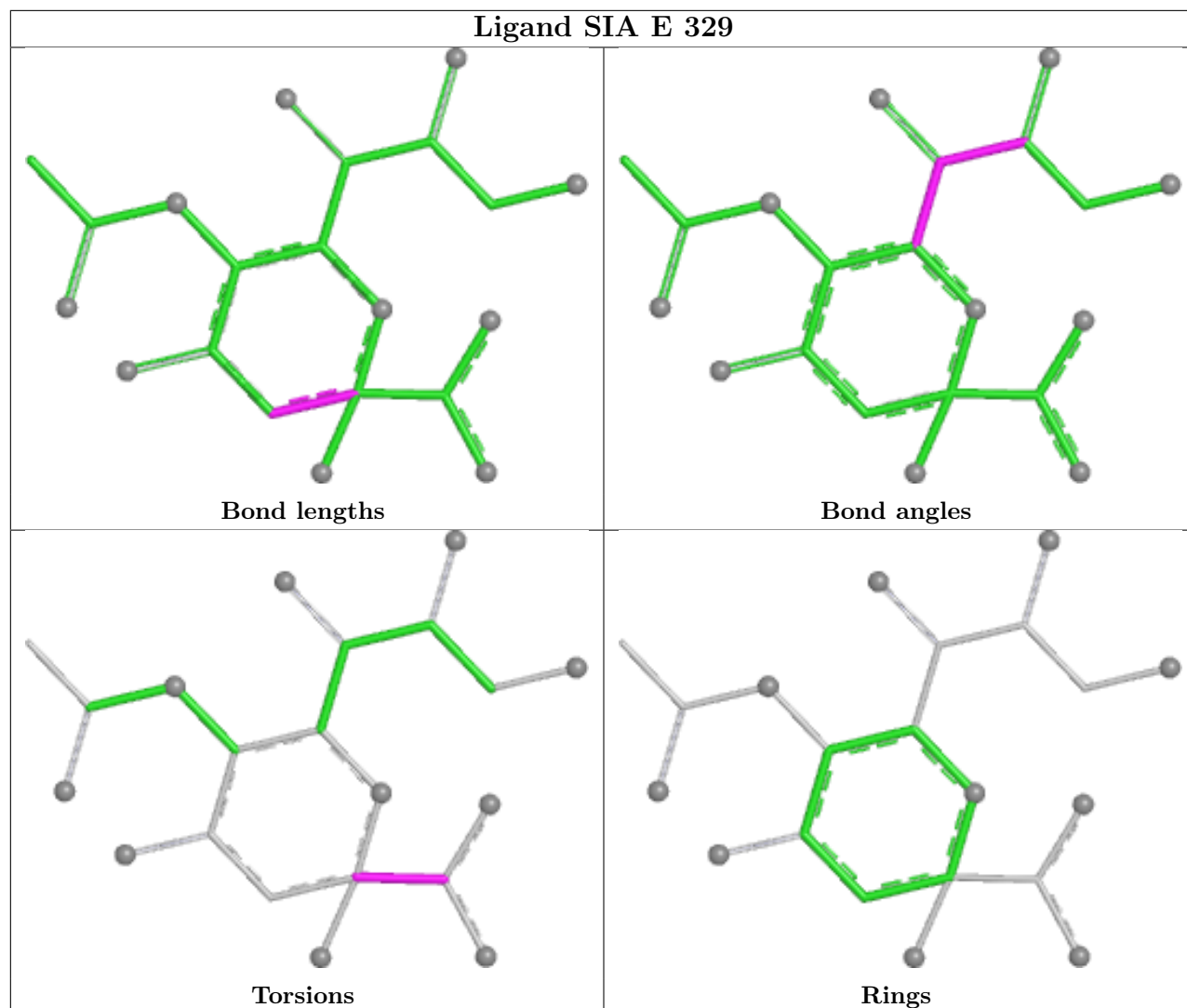


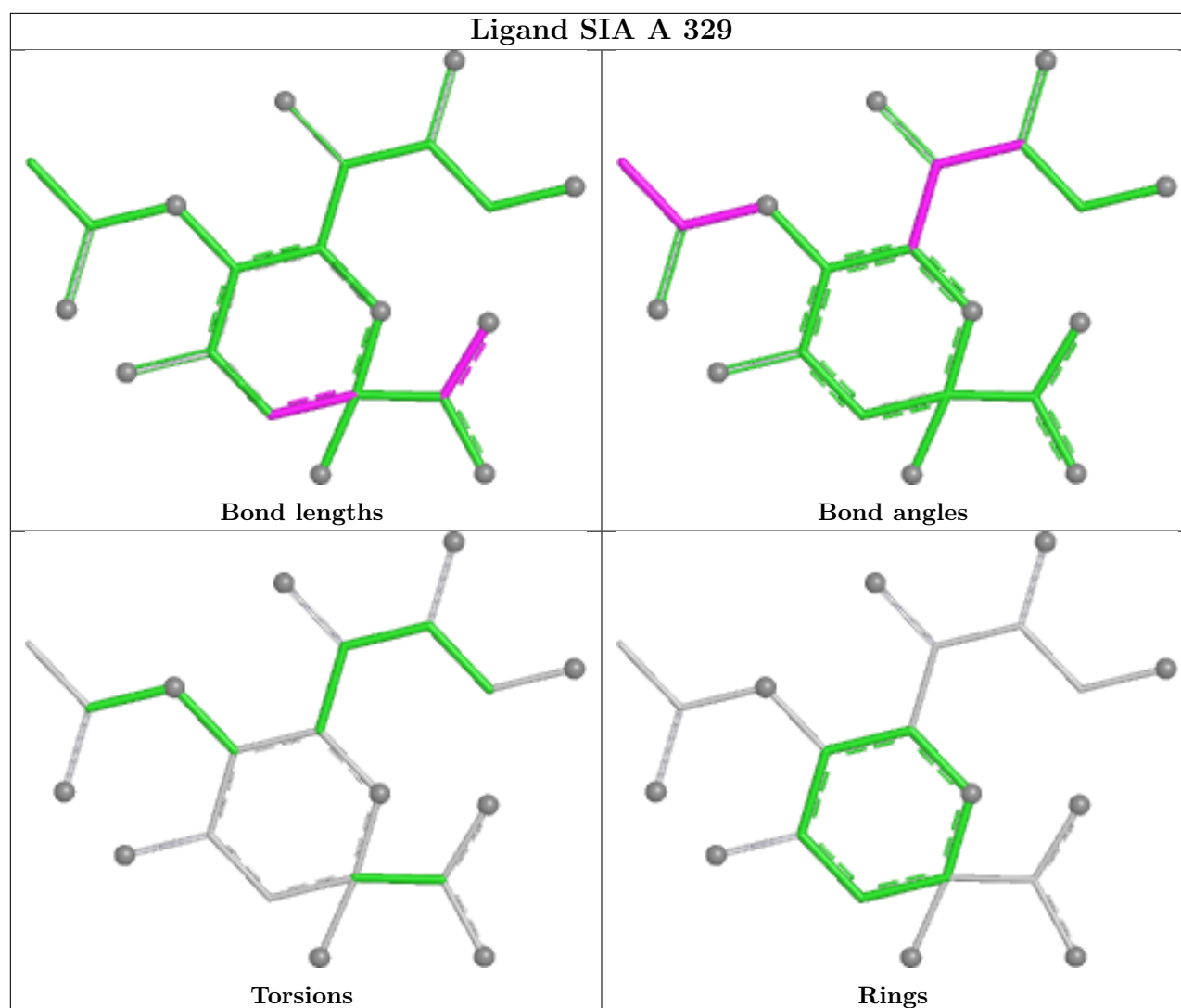
Torsions



Rings

Ligand SIA E 329





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	328/328 (100%)	-0.25	9 (2%) 56 36	3, 22, 51, 133	0
1	C	328/328 (100%)	-0.21	16 (4%) 35 22	2, 21, 47, 129	0
1	E	328/328 (100%)	-0.37	11 (3%) 48 30	3, 21, 46, 131	0
2	B	175/175 (100%)	-0.29	3 (1%) 69 49	2, 16, 47, 98	0
2	D	175/175 (100%)	-0.40	2 (1%) 78 61	2, 15, 46, 99	0
2	F	175/175 (100%)	-0.41	4 (2%) 61 41	2, 15, 46, 98	0
All	All	1509/1509 (100%)	-0.31	45 (2%) 52 33	2, 20, 50, 133	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	GLY	6.5
1	C	6	ASN	5.5
2	F	175	GLY	5.2
1	E	5	GLY	5.0
2	D	175	GLY	4.9
1	C	5	GLY	4.8
1	C	4	PRO	4.8
1	E	144	GLY	4.2
1	E	2	ASP	3.9
1	A	1	GLN	3.9
1	A	8	ASN	3.9
2	B	175	GLY	3.6
1	C	3	LEU	3.4
1	A	3	LEU	3.3
1	E	4	PRO	3.3
1	E	1	GLN	3.2
1	E	328	THR	3.2
1	C	2	ASP	3.2
1	C	328	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	6	ASN	3.1
1	E	3	LEU	3.0
1	C	216	ASN	3.0
1	A	326	LYS	3.0
1	C	8	ASN	3.0
1	E	7	ASP	3.0
1	C	1	GLN	3.0
1	C	240	GLY	2.7
1	A	4	PRO	2.7
2	B	145	ASP	2.7
2	F	58	LYS	2.6
2	F	174	LYS	2.5
2	D	60	ASN	2.3
1	E	291	ASP	2.3
1	C	327	GLN	2.3
1	C	126	THR	2.2
1	C	189	GLN	2.1
1	E	186	SER	2.1
1	C	144	GLY	2.1
1	C	142	GLY	2.1
2	F	173	ILE	2.1
2	B	60	ASN	2.1
1	A	143	PRO	2.1
1	C	7	ASP	2.1
1	E	6	ASN	2.0
1	A	2	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

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

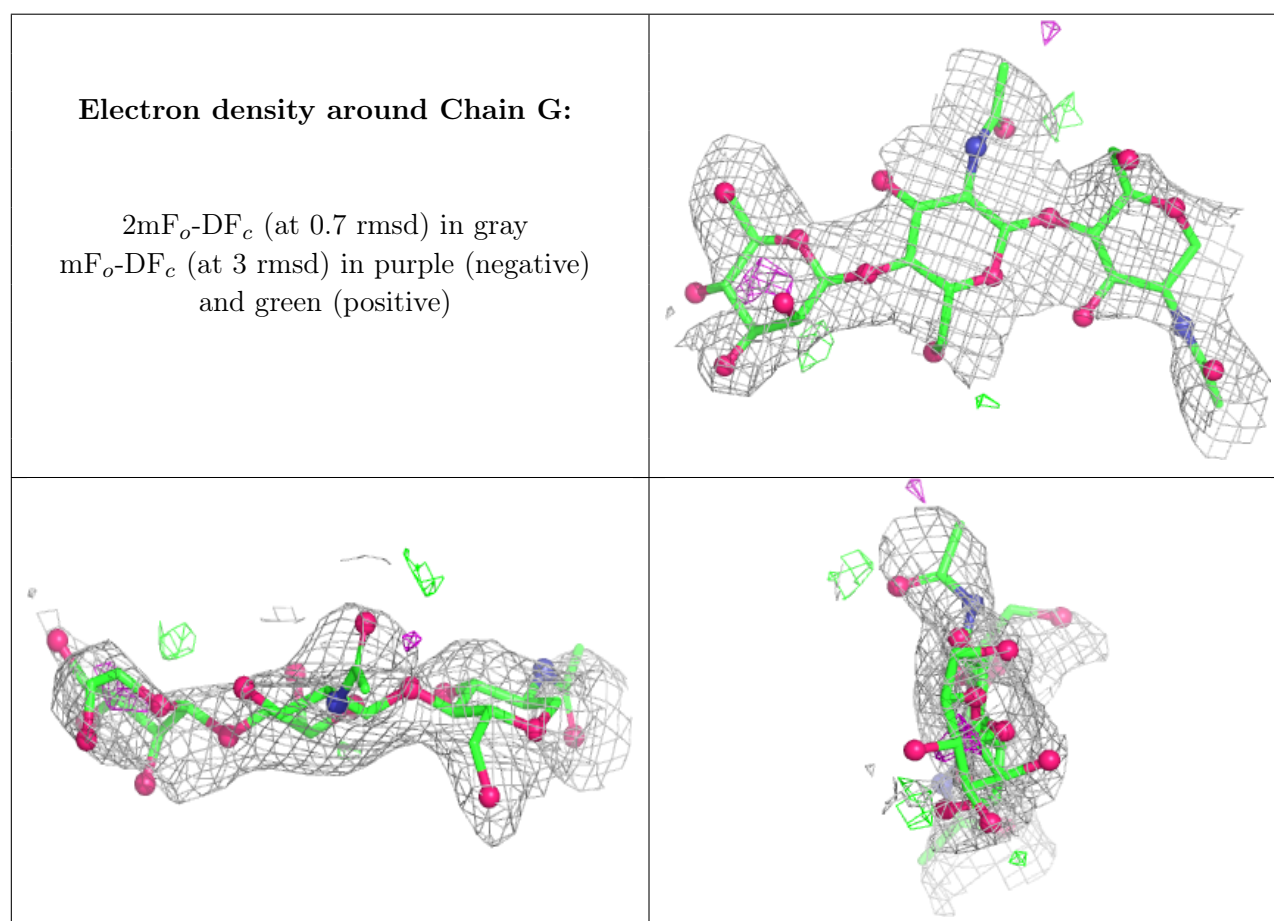
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	G	3	11/12	0.63	0.20	57,59,60,60	0
3	NAG	H	1	14/15	0.79	0.15	38,42,44,45	0

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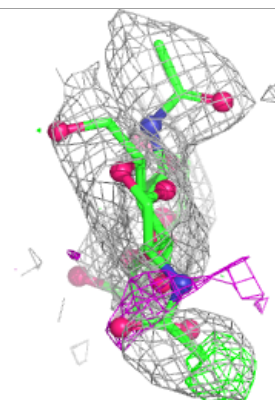
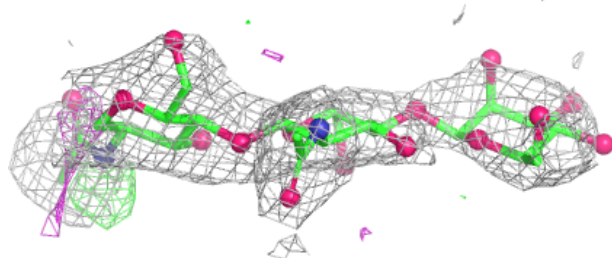
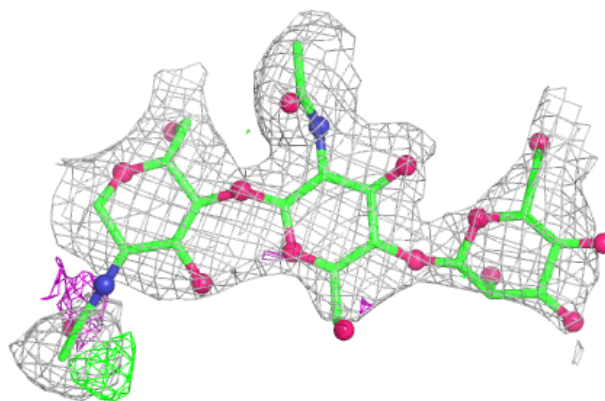
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	H	2	14/15	0.79	0.14	48,50,54,56	0
3	MAN	I	3	11/12	0.82	0.15	59,61,63,64	0
3	NAG	G	2	14/15	0.88	0.11	48,51,54,54	0
3	NAG	I	2	14/15	0.90	0.11	48,51,53,55	0
3	MAN	H	3	11/12	0.90	0.15	60,62,64,65	0
3	NAG	G	1	14/15	0.92	0.11	38,41,43,45	0
3	NAG	I	1	14/15	0.96	0.08	37,40,41,44	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.

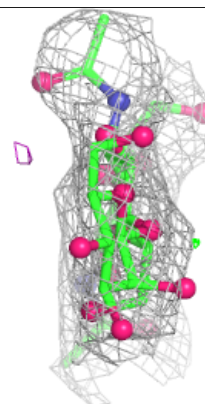
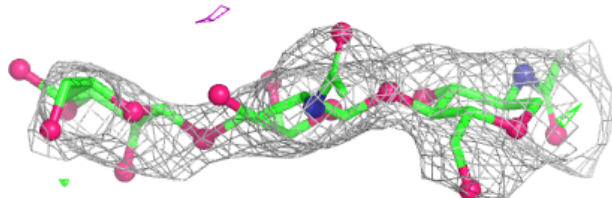
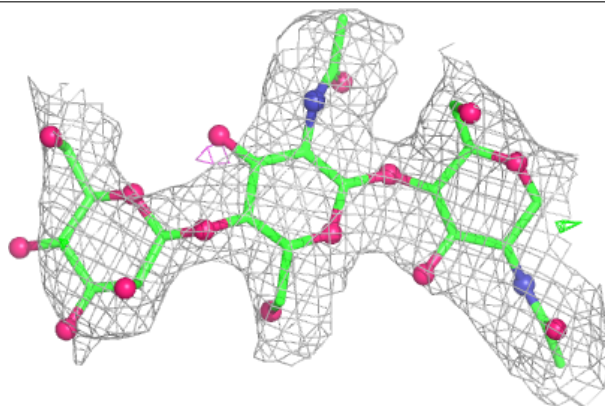


Electron density around Chain H:

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

**Electron density around Chain I:**

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



6.4 Ligands ⓘ

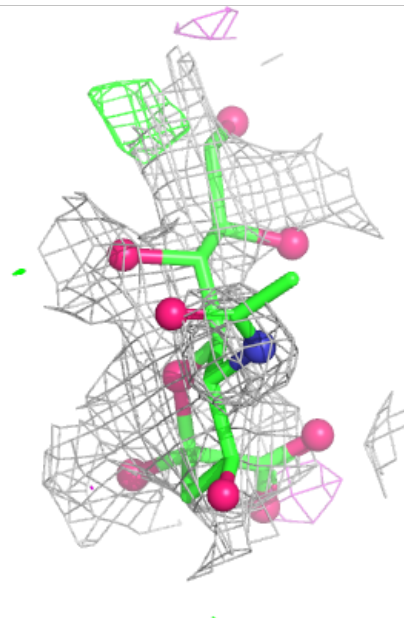
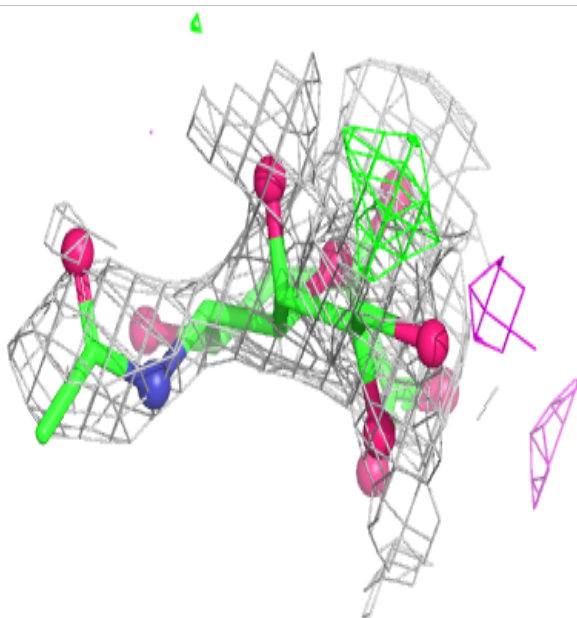
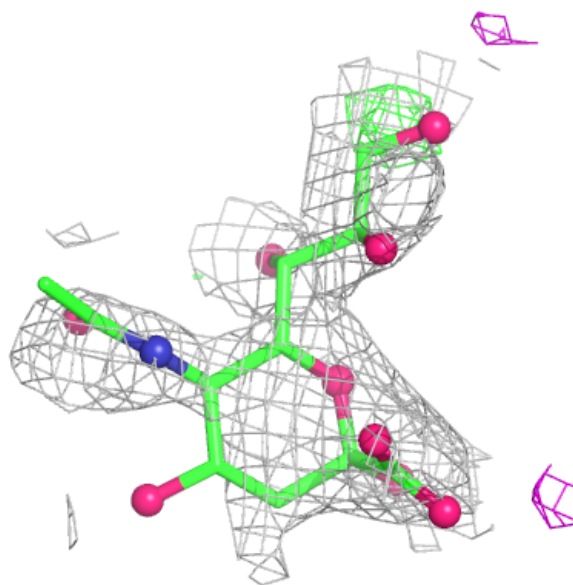
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	F	401	14/15	0.74	0.16	50,54,56,56	0
5	NAG	A	330	14/15	0.77	0.20	38,42,44,44	0
5	NAG	A	334	14/15	0.79	0.13	37,41,42,43	0
5	NAG	E	334	14/15	0.80	0.13	38,40,43,44	0
4	SIA	A	329	21/21	0.80	0.21	49,49,50,50	21
5	NAG	D	401	14/15	0.81	0.16	51,55,56,57	0
5	NAG	E	330	14/15	0.81	0.18	39,43,44,44	0
4	SIA	C	329	21/21	0.82	0.23	49,50,50,50	21
5	NAG	E	348	14/15	0.83	0.15	36,40,42,42	0
5	NAG	A	348	14/15	0.83	0.12	34,39,40,40	0
5	NAG	C	334	14/15	0.84	0.13	38,41,42,43	0
4	SIA	E	329	21/21	0.84	0.21	49,49,50,50	21
5	NAG	B	401	14/15	0.84	0.15	51,54,56,56	0
5	NAG	C	348	14/15	0.90	0.12	35,39,41,42	0
5	NAG	C	330	14/15	0.90	0.11	38,41,43,43	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.

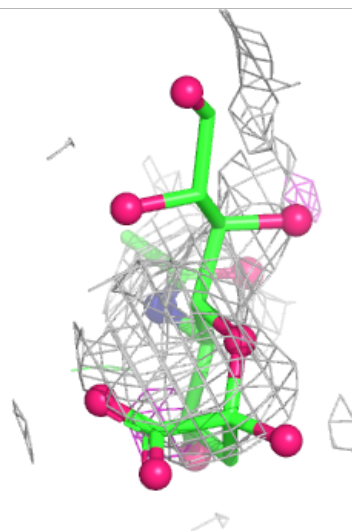
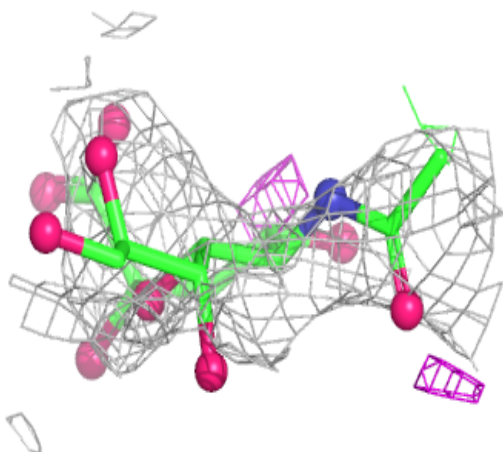
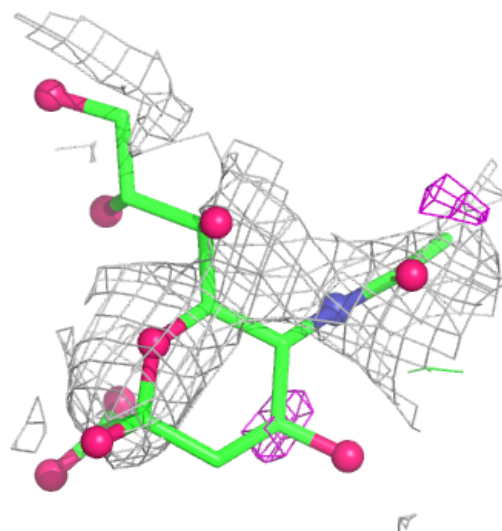
Electron density around SIA A 329:

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



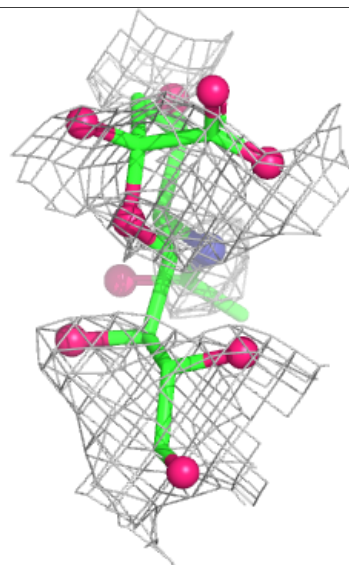
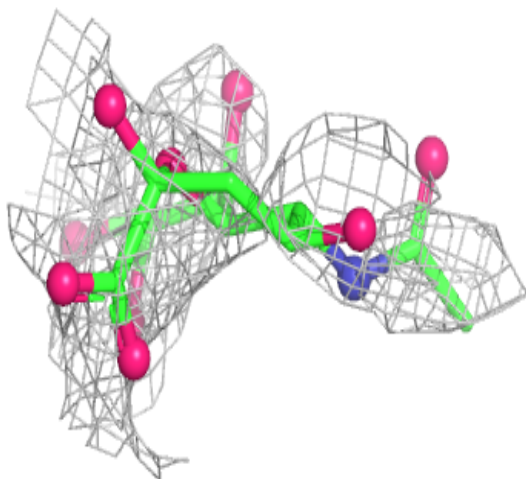
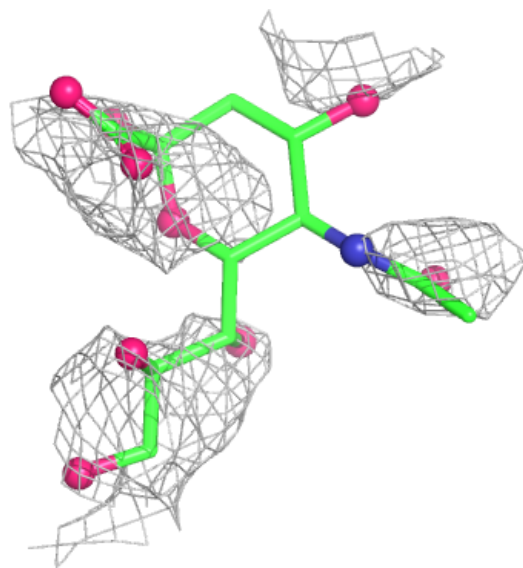
Electron density around SIA C 329:

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 SIA E 329:

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.