Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 07:32 PM BST

PDB ID	:	5HMG
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 following versions of software and data (see references ⓘ) were used in the production of this report:

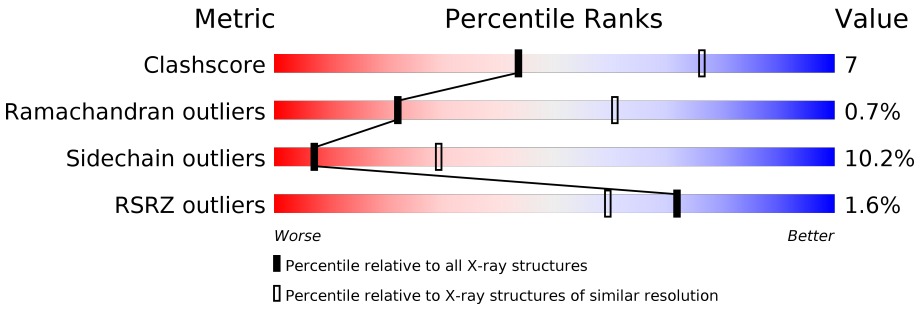
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	328	2% 72% 24% •
1	C	328	2% 72% 24% • •
1	E	328	2% 73% 24% •
2	B	175	% 70% 25% • •
2	D	175	% 70% 26% • •
2	F	175	% 73% 23% • •
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

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			

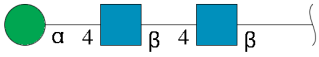
- Molecule 2 is a protein called Hemagglutinin HA2 chain.

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:

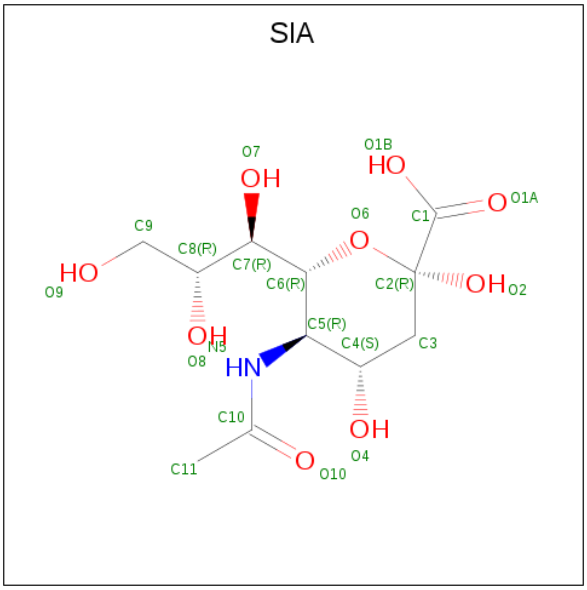
Chain	Residue	Modelled	Actual	Comment	Reference
B	112	GLY	ASP	conflict	UNP P03437
D	112	GLY	ASP	conflict	UNP P03437
F	112	GLY	ASP	conflict	UNP P03437

- 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.



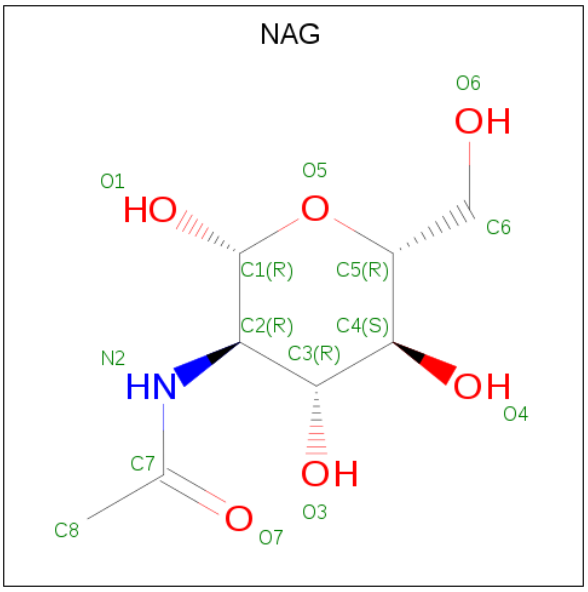
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	G	3	Total C N O 39 22 2 15	0	0	0
3	H	3	Total C N O 39 22 2 15	0	0	0
3	I	3	Total C N O 39 22 2 15	0	0	0

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



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

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



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

- Molecule 6 is water.

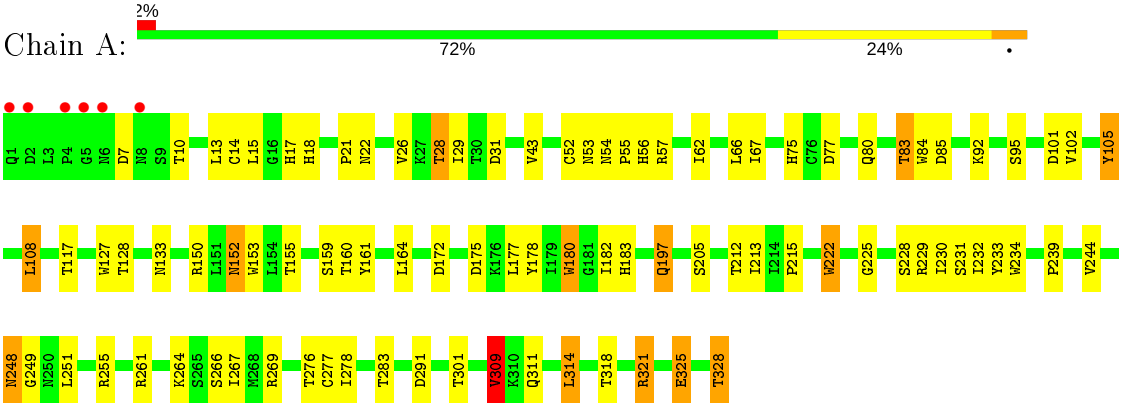
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	8	Total O 8 8	0	0
6	B	5	Total O 5 5	0	0
6	C	8	Total O 8 8	0	0
6	D	5	Total O 5 5	0	0
6	E	9	Total O 9 9	0	0
6	F	4	Total O 4 4	0	0

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.

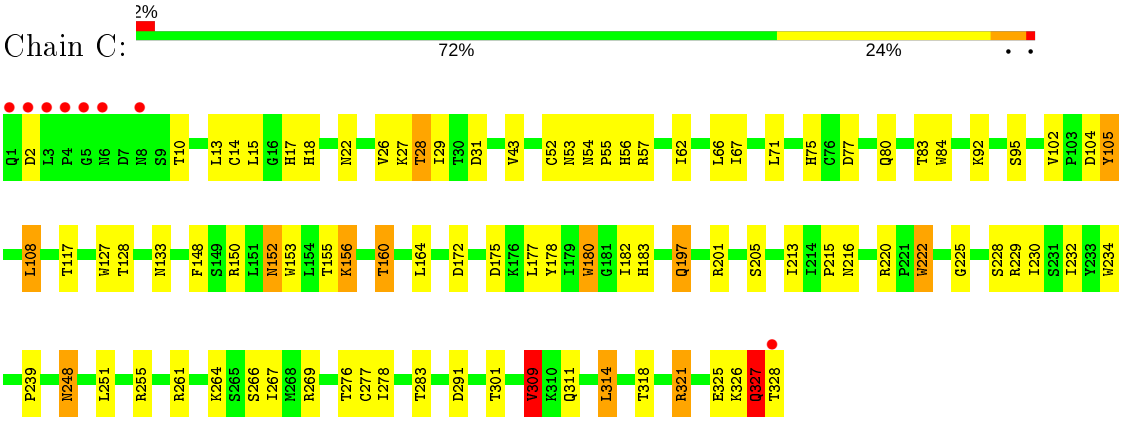
- Molecule 1: Hemagglutinin HA1 chain

Chain A:



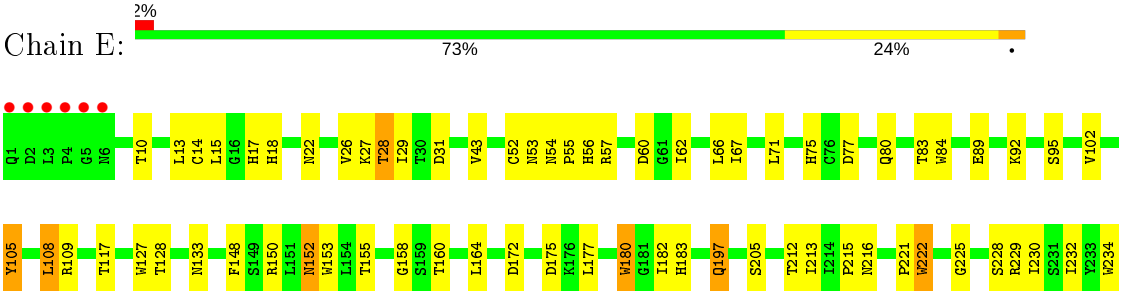
- Molecule 1: Hemagglutinin HA1 chain

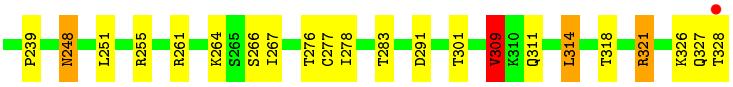
Chain C:



- Molecule 1: Hemagglutinin HA1 chain

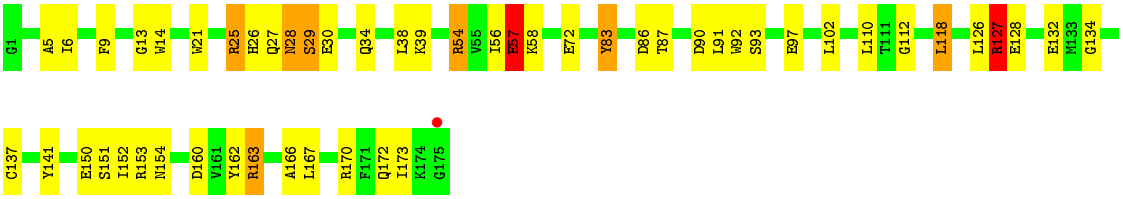
Chain E:





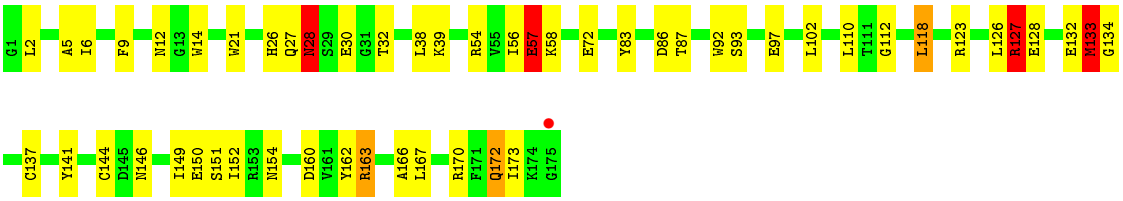
• Molecule 2: Hemagglutinin HA2 chain

Chain B:



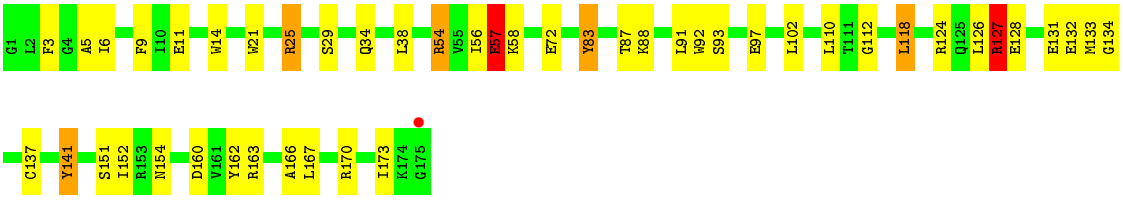
• Molecule 2: Hemagglutinin HA2 chain

Chain D:



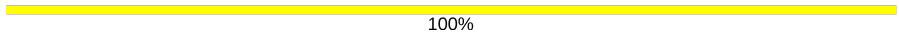
• Molecule 2: Hemagglutinin HA2 chain

Chain F:



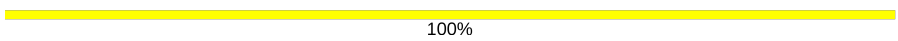
• Molecule 3: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



• 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:



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

Chain I:

4 Data and refinement statistics (i)

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 7.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-3.20) 78.9 (7.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.220 , (Not available) 0.208 , (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)	0.24 , 46.7	EDS
L-test for twinning[1]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	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.*

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, NAG, 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	0.86	0/2589	1.41	29/3527 (0.8%)
1	C	0.87	0/2589	1.43	32/3527 (0.9%)
1	E	0.88	0/2589	1.40	28/3527 (0.8%)
2	B	0.91	0/1441	1.48	22/1933 (1.1%)
2	D	0.93	0/1441	1.47	24/1933 (1.2%)
2	F	0.92	0/1441	1.47	22/1933 (1.1%)
All	All	0.89	0/12090	1.44	157/16380 (1.0%)

There are no bond length outliers.

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	255	ARG	NE-CZ-NH1	-9.95	115.32	120.30
2	B	170	ARG	NE-CZ-NH1	-9.36	115.62	120.30
2	B	25	ARG	NE-CZ-NH1	-9.35	115.63	120.30
1	A	255	ARG	NE-CZ-NH1	-9.12	115.74	120.30
1	C	321	ARG	NE-CZ-NH1	-9.09	115.75	120.30
2	B	92	TRP	CD1-CG-CD2	9.06	113.55	106.30
1	E	255	ARG	NE-CZ-NH1	-8.87	115.86	120.30
1	C	180	TRP	CD1-CG-CD2	8.69	113.25	106.30
1	A	180	TRP	CD1-CG-CD2	8.57	113.16	106.30
1	A	127	TRP	CD1-CG-CD2	8.56	113.15	106.30
1	A	321	ARG	NE-CZ-NH1	-8.52	116.04	120.30
1	C	127	TRP	CD1-CG-CD2	8.51	113.11	106.30
2	D	92	TRP	CD1-CG-CD2	8.35	112.98	106.30
1	E	84	TRP	CD1-CG-CD2	8.34	112.98	106.30
2	F	14	TRP	CD1-CG-CD2	8.22	112.88	106.30
1	E	127	TRP	CD1-CG-CD2	8.14	112.81	106.30
1	A	105	TYR	CB-CG-CD2	-8.06	116.17	121.00
2	D	14	TRP	CD1-CG-CD2	8.06	112.75	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	180	TRP	CD1-CG-CD2	8.02	112.72	106.30
1	E	222	TRP	CD1-CG-CD2	8.00	112.70	106.30
2	F	92	TRP	CD1-CG-CD2	7.99	112.69	106.30
1	A	222	TRP	CD1-CG-CD2	7.97	112.68	106.30
1	A	180	TRP	CE2-CD2-CG	-7.95	100.94	107.30
2	D	21	TRP	CD1-CG-CD2	7.88	112.61	106.30
1	C	153	TRP	CD1-CG-CD2	7.87	112.59	106.30
1	C	180	TRP	CE2-CD2-CG	-7.82	101.05	107.30
2	B	14	TRP	CD1-CG-CD2	7.78	112.52	106.30
1	C	222	TRP	CD1-CG-CD2	7.77	112.51	106.30
2	D	170	ARG	NE-CZ-NH1	-7.71	116.44	120.30
1	C	84	TRP	CD1-CG-CD2	7.64	112.41	106.30
1	E	84	TRP	CE2-CD2-CG	-7.59	101.23	107.30
1	A	84	TRP	CD1-CG-CD2	7.56	112.35	106.30
2	D	14	TRP	CE2-CD2-CG	-7.51	101.29	107.30
2	B	21	TRP	CD1-CG-CD2	7.49	112.29	106.30
2	F	21	TRP	CD1-CG-CD2	7.46	112.26	106.30
2	B	92	TRP	CE2-CD2-CG	-7.45	101.34	107.30
1	A	234	TRP	CD1-CG-CD2	7.41	112.23	106.30
2	D	92	TRP	CE2-CD2-CG	-7.39	101.39	107.30
1	E	180	TRP	CE2-CD2-CG	-7.38	101.39	107.30
1	E	127	TRP	CE2-CD2-CG	-7.36	101.42	107.30
2	F	170	ARG	NE-CZ-NH1	-7.36	116.62	120.30
1	A	127	TRP	CE2-CD2-CG	-7.34	101.43	107.30
2	B	14	TRP	CE2-CD2-CG	-7.33	101.44	107.30
1	E	321	ARG	NE-CZ-NH1	-7.32	116.64	120.30
1	C	127	TRP	CE2-CD2-CG	-7.31	101.45	107.30
1	C	84	TRP	CE2-CD2-CG	-7.28	101.47	107.30
1	A	153	TRP	CD1-CG-CD2	7.27	112.12	106.30
2	B	21	TRP	CE2-CD2-CG	-7.19	101.55	107.30
1	E	105	TYR	CB-CG-CD2	-7.17	116.70	121.00
1	E	234	TRP	CD1-CG-CD2	7.12	112.00	106.30
1	A	84	TRP	CE2-CD2-CG	-7.10	101.62	107.30
1	E	222	TRP	CE2-CD2-CG	-7.06	101.65	107.30
1	E	177	LEU	CA-CB-CG	7.03	131.47	115.30
1	C	234	TRP	CD1-CG-CD2	6.99	111.89	106.30
1	A	222	TRP	CE2-CD2-CG	-6.97	101.72	107.30
2	F	14	TRP	CE2-CD2-CG	-6.95	101.74	107.30
1	C	177	LEU	CA-CB-CG	6.92	131.21	115.30
1	E	153	TRP	CD1-CG-CD2	6.91	111.83	106.30
1	C	222	TRP	CE2-CD2-CG	-6.90	101.78	107.30
2	F	127	ARG	CA-CB-CG	-6.87	98.28	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	234	TRP	CE2-CD2-CG	-6.83	101.83	107.30
2	D	127	ARG	CA-CB-CG	-6.83	98.37	113.40
1	C	105	TYR	CB-CG-CD2	-6.81	116.92	121.00
2	F	21	TRP	CE2-CD2-CG	-6.80	101.86	107.30
2	B	127	ARG	CA-CB-CG	-6.80	98.44	113.40
2	D	21	TRP	CE2-CD2-CG	-6.80	101.86	107.30
2	F	92	TRP	CE2-CD2-CG	-6.79	101.87	107.30
1	A	177	LEU	CA-CB-CG	6.75	130.82	115.30
1	C	153	TRP	CE2-CD2-CG	-6.75	101.90	107.30
2	B	92	TRP	CG-CD2-CE3	6.73	139.96	133.90
1	A	153	TRP	CE2-CD2-CG	-6.72	101.93	107.30
2	B	25	ARG	NE-CZ-NH2	6.69	123.64	120.30
1	E	234	TRP	CE2-CD2-CG	-6.69	101.95	107.30
2	D	172	GLN	CA-CB-CG	6.61	127.93	113.40
2	D	57	GLU	CA-CB-CG	6.56	127.84	113.40
2	B	57	GLU	CA-CB-CG	6.54	127.79	113.40
2	F	57	GLU	CA-CB-CG	6.52	127.75	113.40
1	C	234	TRP	CE2-CD2-CG	-6.38	102.19	107.30
2	B	83	TYR	CB-CG-CD2	-6.33	117.20	121.00
2	F	83	TYR	CB-CG-CD2	-6.29	117.23	121.00
2	D	92	TRP	CG-CD2-CE3	6.18	139.46	133.90
2	B	92	TRP	CG-CD1-NE1	-6.14	103.95	110.10
2	F	110	LEU	CA-CB-CG	6.11	129.34	115.30
2	D	110	LEU	CA-CB-CG	6.00	129.11	115.30
2	F	14	TRP	CG-CD2-CE3	5.97	139.28	133.90
2	F	162	TYR	CB-CG-CD2	-5.97	117.42	121.00
2	D	14	TRP	CG-CD2-CE3	5.96	139.26	133.90
1	E	153	TRP	CE2-CD2-CG	-5.93	102.56	107.30
2	F	92	TRP	CG-CD2-CE3	5.91	139.22	133.90
2	B	14	TRP	CG-CD2-CE3	5.91	139.22	133.90
1	C	127	TRP	CG-CD1-NE1	-5.90	104.20	110.10
1	E	28	THR	CA-CB-CG2	5.89	120.64	112.40
2	D	92	TRP	CG-CD1-NE1	-5.87	104.23	110.10
1	E	309	VAL	N-CA-CB	-5.85	98.62	111.50
1	C	22	ASN	CA-C-N	5.80	127.80	116.20
2	B	110	LEU	CA-CB-CG	5.79	128.61	115.30
2	D	83	TYR	CB-CG-CD2	-5.78	117.53	121.00
2	F	92	TRP	CG-CD1-NE1	-5.77	104.33	110.10
2	D	28	ASN	CB-CG-ND2	5.72	130.42	116.70
1	C	28	THR	CA-CB-CG2	5.72	120.40	112.40
1	A	22	ASN	CA-C-N	5.71	127.63	116.20
1	E	255	ARG	NE-CZ-NH2	5.70	123.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	309	VAL	N-CA-CB	-5.67	99.02	111.50
1	C	153	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	A	28	THR	CA-CB-CG2	5.64	120.30	112.40
1	A	178	TYR	CB-CG-CD2	-5.61	117.63	121.00
1	C	255	ARG	NE-CZ-NH2	5.59	123.09	120.30
1	E	180	TRP	CG-CD2-CE3	5.58	138.92	133.90
1	C	178	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	C	269	ARG	NE-CZ-NH1	-5.53	117.54	120.30
2	F	14	TRP	CG-CD1-NE1	-5.50	104.60	110.10
2	D	162	TYR	CB-CG-CD2	-5.49	117.71	121.00
2	F	133	MET	CB-CG-SD	-5.48	95.97	112.40
1	E	60	ASP	CB-CG-OD2	5.46	123.22	118.30
2	F	25	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	C	180	TRP	CG-CD1-NE1	-5.46	104.64	110.10
2	D	163	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	A	127	TRP	CG-CD1-NE1	-5.43	104.67	110.10
2	D	86	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	180	TRP	CG-CD2-CE3	5.41	138.77	133.90
2	D	133	MET	CA-CB-CG	5.41	122.50	113.30
1	C	104	ASP	CB-CG-OD1	5.40	123.16	118.30
2	B	163	ARG	NE-CZ-NH1	-5.37	117.61	120.30
2	F	21	TRP	CG-CD1-NE1	-5.32	104.78	110.10
1	E	153	TRP	CG-CD1-NE1	-5.32	104.78	110.10
2	B	90	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	85	ASP	CB-CG-OD1	5.25	123.02	118.30
2	D	92	TRP	CB-CG-CD1	-5.25	120.18	127.00
1	E	84	TRP	CG-CD2-CE3	5.25	138.62	133.90
1	A	127	TRP	CB-CG-CD1	-5.24	120.19	127.00
1	A	180	TRP	CG-CD1-NE1	-5.22	104.88	110.10
1	E	84	TRP	CG-CD1-NE1	-5.22	104.88	110.10
2	B	86	ASP	CB-CG-OD1	5.21	122.99	118.30
1	E	180	TRP	CG-CD1-NE1	-5.20	104.90	110.10
2	F	124	ARG	NE-CZ-NH1	-5.20	117.70	120.30
2	B	27	GLN	N-CA-C	-5.19	96.98	111.00
1	A	309	VAL	N-CA-CB	-5.17	100.14	111.50
1	C	127	TRP	CB-CG-CD1	-5.17	120.28	127.00
1	E	28	THR	N-CA-CB	-5.12	100.56	110.30
1	E	222	TRP	CG-CD1-NE1	-5.11	104.99	110.10
2	B	14	TRP	CG-CD1-NE1	-5.11	104.99	110.10
1	C	180	TRP	CG-CD2-CE3	5.10	138.49	133.90
1	A	28	THR	N-CA-CB	-5.09	100.62	110.30
1	C	180	TRP	CB-CG-CD1	-5.08	120.40	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	123	ARG	NE-CZ-NH2	-5.08	117.76	120.30
2	D	21	TRP	CG-CD1-NE1	-5.07	105.03	110.10
2	B	162	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	A	269	ARG	NE-CZ-NH1	-5.05	117.77	120.30
1	C	327	GLN	CA-CB-CG	5.05	124.52	113.40
1	E	22	ASN	CA-C-N	5.05	126.30	116.20
1	A	180	TRP	CB-CG-CD1	-5.05	120.44	127.00
1	A	83	THR	N-CA-CB	-5.04	100.72	110.30
2	D	14	TRP	CG-CD1-NE1	-5.04	105.06	110.10
1	C	222	TRP	CG-CD1-NE1	-5.04	105.06	110.10
1	C	201	ARG	NE-CZ-NH1	-5.03	117.79	120.30
2	F	83	TYR	CD1-CE1-CZ	-5.01	115.29	119.80
2	F	141	TYR	CB-CG-CD2	-5.01	118.00	121.00

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	28	0
2	D	1417	0	1344	28	0
2	F	1417	0	1344	25	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	161	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 (161) 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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE21	2:D:97:GLU:HB2	1.77	0.48
1:C:311:GLN:NE2	2:D:97:GLU:HB2	2.29	0.48
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:180:TRP:CH2	1:E:213:ILE:HD13	2.49	0.47
1:E:54:ASN:O	1:E:278:ILE:HA	2.14	0.47
1:A:117:THR:HG21	1:A:261:ARG:HH21	1.80	0.47
1:A:102:VAL:HG22	1:A:232:ILE:HB	1.96	0.47
2:F:163:ARG:O	2:F:167:LEU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:133:ASN:H	1:A:152:ASN:ND2	2.13	0.46
1:A:54:ASN:O	1:A:278:ILE:HA	2.16	0.46
1:E:15:LEU:HD23	2:F:118:LEU:HD13	1.97	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:A:212:THR:HG21	1:E:216:ASN:HB3	1.98	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
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:182:ILE:HD11	1:C:215:PRO:HD3	2.00	0.43
1:C:52:CYS:HB3	1:C:277:CYS:O	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:71:LEU:O	1:E:148:PHE:HB3	2.18	0.43
1:E:43:VAL:HG23	1:E:314:LEU:HB2	1.99	0.43
1:C:228:SER:O	1:C:229:ARG:HD2	2.18	0.43
1:C:43:VAL:HG23	1:C:314:LEU:HB2	2.00	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:HB3	2:B:39:LYS:HE2	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
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:309:VAL:HG22	2:D:93:SER:HA	2.03	0.41
1:C:71:LEU:O	1:C:148:PHE:HB3	2.20	0.41
1:C:102:VAL:HB	1:C:105:TYR:HD2	1.85	0.41
2:D:39:LYS:HE2	2:D:39:LYS:HB3	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
1:C:53:ASN:OD1	1:C:276:THR:HA	2.21	0.41
2:B:127:ARG:NH2	2:F:131:GLU:OE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:ALA:HA	2:B:9:PHE:CE2	2.56	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:C:216:ASN:HB2	1:C:220:ARG:HH12	1.87	0.40
1:A:244:VAL:CG2	1:E:221:PRO:HG3	2.51	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: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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	326/328 (99%)	307 (94%)	18 (6%)	1 (0%)	41 74
1	C	326/328 (99%)	311 (95%)	13 (4%)	2 (1%)	25 64
1	E	326/328 (99%)	312 (96%)	12 (4%)	2 (1%)	25 64
2	B	173/175 (99%)	161 (93%)	9 (5%)	3 (2%)	9 42
2	D	173/175 (99%)	162 (94%)	10 (6%)	1 (1%)	25 64
2	F	173/175 (99%)	163 (94%)	9 (5%)	1 (1%)	25 64
All	All	1497/1509 (99%)	1416 (95%)	71 (5%)	10 (1%)	22 61

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 (i)

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%)	258 (89%)	31 (11%)	6 27
1	E	289/289 (100%)	258 (89%)	31 (11%)	6 27
2	B	148/148 (100%)	134 (90%)	14 (10%)	8 32
2	D	148/148 (100%)	134 (90%)	14 (10%)	8 32
2	F	148/148 (100%)	136 (92%)	12 (8%)	11 42
All	All	1311/1311 (100%)	1177 (90%)	134 (10%)	7 29

All (134) 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	55	PRO
1	A	57	ARG
1	A	75	HIS

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Mol	Chain	Res	Type
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	152	ASN
1	A	159	SER
1	A	160	THR
1	A	164	LEU
1	A	172	ASP
1	A	197	GLN
1	A	205	SER
1	A	248	ASN
1	A	251	LEU
1	A	266	SER
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	54	ARG
2	B	56	ILE
2	B	57	GLU
2	B	72	GLU
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
1	C	2	ASP
1	C	13	LEU
1	C	18	HIS
1	C	26	VAL
1	C	28	THR

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Mol	Chain	Res	Type
1	C	31	ASP
1	C	55	PRO
1	C	57	ARG
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	152	ASN
1	C	156	LYS
1	C	160	THR
1	C	164	LEU
1	C	172	ASP
1	C	197	GLN
1	C	205	SER
1	C	248	ASN
1	C	251	LEU
1	C	266	SER
1	C	291	ASP
1	C	309	VAL
1	C	314	LEU
1	C	318	THR
1	C	321	ARG
1	C	327	GLN
2	D	28	ASN
2	D	38	LEU
2	D	54	ARG
2	D	56	ILE
2	D	57	GLU
2	D	72	GLU
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	172	GLN
2	D	173	ILE
1	E	13	LEU
1	E	18	HIS

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Mol	Chain	Res	Type
1	E	26	VAL
1	E	28	THR
1	E	31	ASP
1	E	55	PRO
1	E	57	ARG
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	150	ARG
1	E	152	ASN
1	E	160	THR
1	E	164	LEU
1	E	172	ASP
1	E	197	GLN
1	E	205	SER
1	E	248	ASN
1	E	251	LEU
1	E	266	SER
1	E	291	ASP
1	E	309	VAL
1	E	314	LEU
1	E	318	THR
1	E	321	ARG
1	E	326	LYS
1	E	327	GLN
1	E	328	THR
2	F	11	GLU
2	F	29	SER
2	F	38	LEU
2	F	54	ARG
2	F	56	ILE
2	F	57	GLU
2	F	72	GLU
2	F	118	LEU
2	F	127	ARG
2	F	128	GLU
2	F	160	ASP
2	F	173	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	248	ASN
2	B	27	GLN
1	C	152	ASN
1	C	248	ASN
1	C	327	GLN
2	D	12	ASN
2	D	49	ASN
1	E	152	ASN
1	E	248	ASN
2	F	49	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

9 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	G	1	1,3	14,14,15	0.78	1 (7%)	17,19,21	0.76	0
3	NAG	G	2	3	14,14,15	0.43	0	17,19,21	0.94	1 (5%)
3	MAN	G	3	3	11,11,12	0.86	0	15,15,17	1.29	2 (13%)
3	NAG	H	1	1,3	14,14,15	0.87	1 (7%)	17,19,21	0.86	1 (5%)
3	NAG	H	2	3	14,14,15	0.48	0	17,19,21	0.94	1 (5%)
3	MAN	H	3	3	11,11,12	0.68	0	15,15,17	1.37	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	I	1	1,3	14,14,15	0.62	0	17,19,21	0.81	1 (5%)
3	NAG	I	2	3	14,14,15	0.49	0	17,19,21	0.97	1 (5%)
3	MAN	I	3	3	11,11,12	0.77	0	15,15,17	1.42	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	1	1,3	-	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	1,3	-	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	1,3	-	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	-2.55	1.39	1.43
3	G	1	NAG	O5-C1	-2.13	1.40	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	3	MAN	C1-O5-C5	3.41	116.81	112.19
3	I	3	MAN	O2-C2-C1	2.94	115.18	109.15
3	I	3	MAN	O5-C1-C2	2.82	115.12	110.77
3	H	3	MAN	O3-C3-C2	2.73	115.22	109.99
3	G	3	MAN	C1-C2-C3	-2.72	106.33	109.67
3	H	2	NAG	C4-C3-C2	-2.53	107.31	111.02
3	I	2	NAG	C4-C3-C2	-2.46	107.42	111.02
3	G	3	MAN	C3-C4-C5	2.30	114.34	110.24
3	G	2	NAG	C4-C3-C2	-2.30	107.65	111.02
3	I	1	NAG	C1-O5-C5	2.18	115.14	112.19
3	H	1	NAG	C1-O5-C5	2.08	115.01	112.19

All (3) chirality outliers are listed below:

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

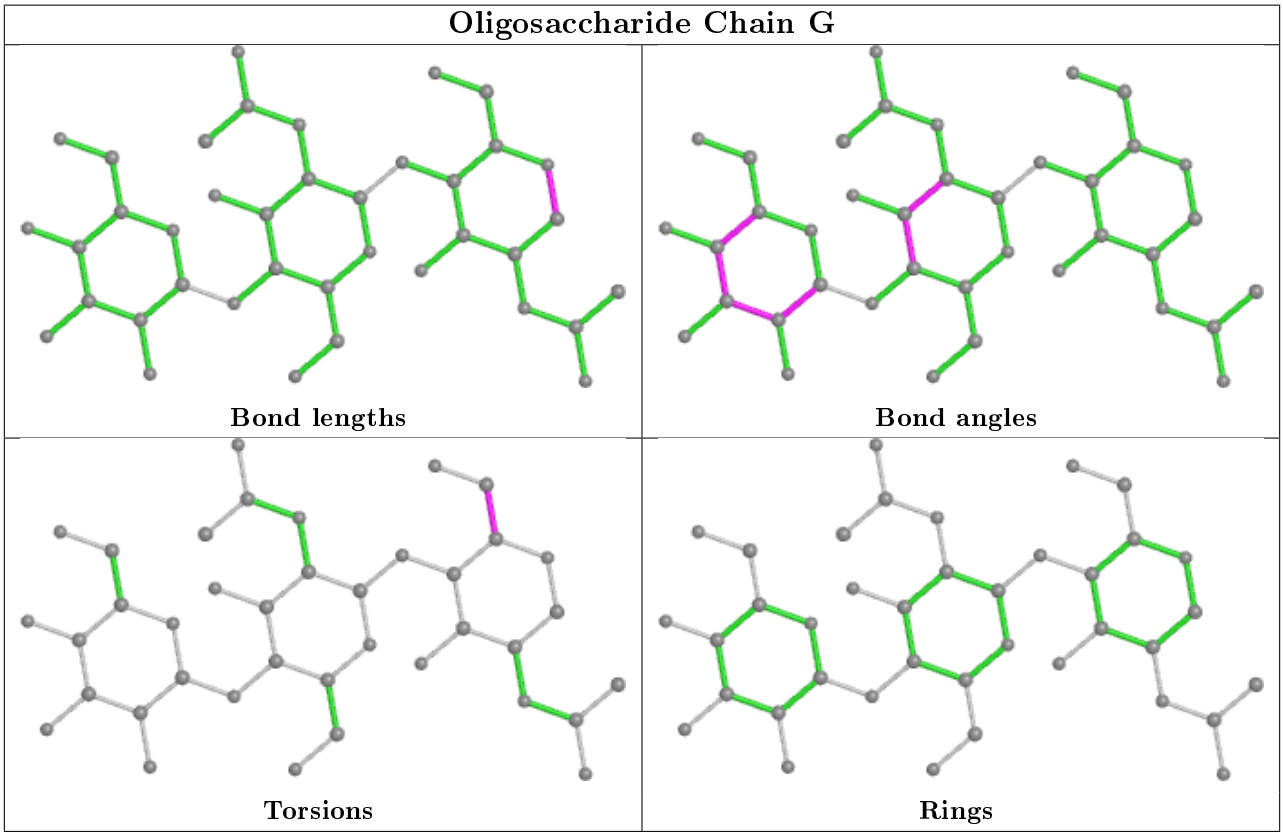
All (6) torsion outliers are listed below:

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

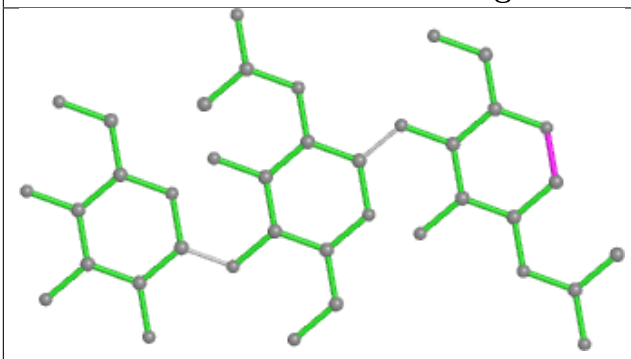
There are no ring outliers.

No monomer is involved in short contacts.

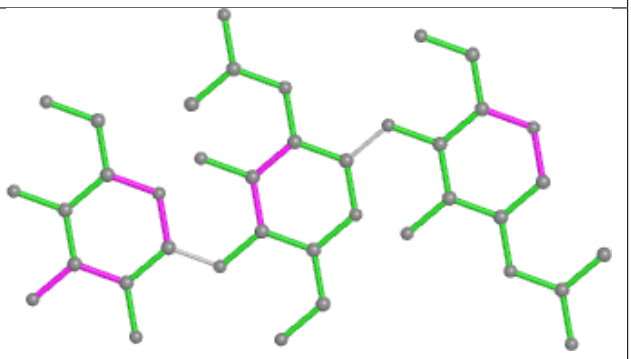
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



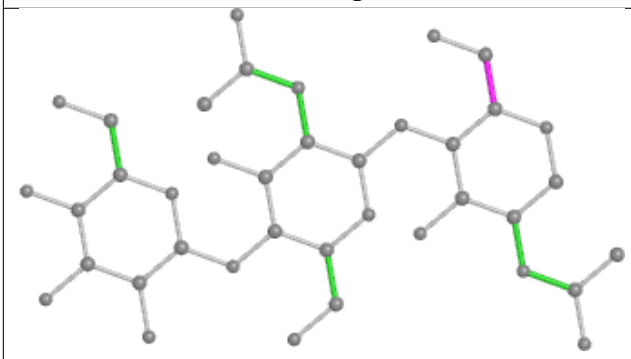
Oligosaccharide Chain H



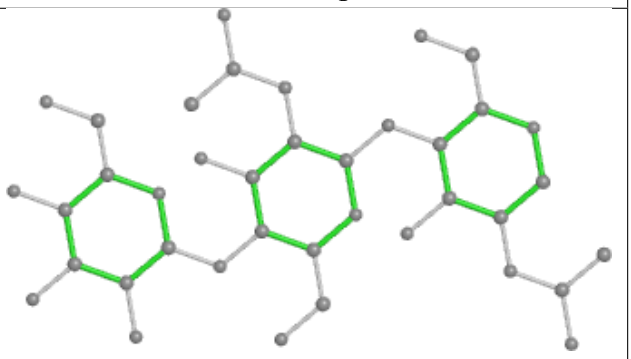
Bond lengths



Bond angles

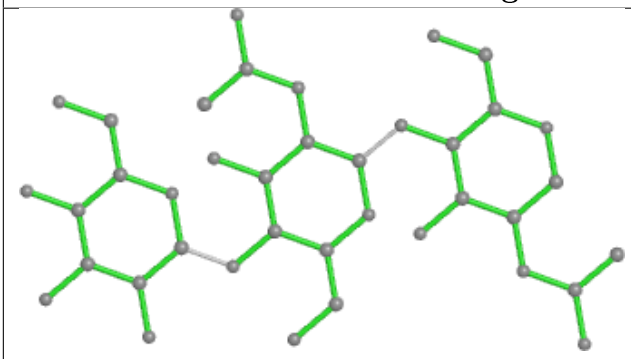


Torsions

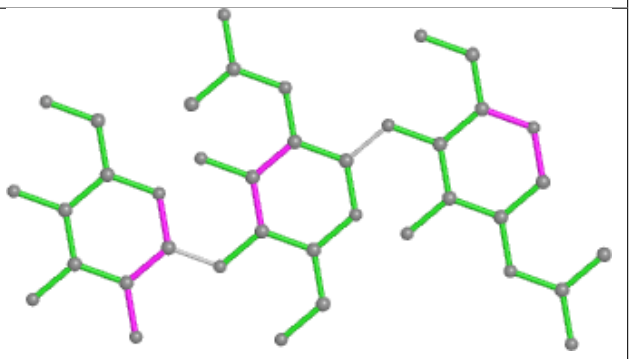


Rings

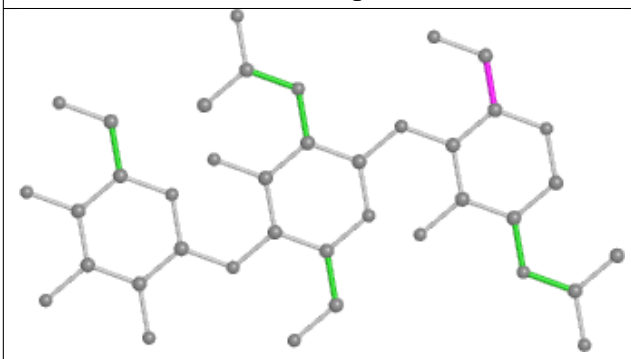
Oligosaccharide Chain I



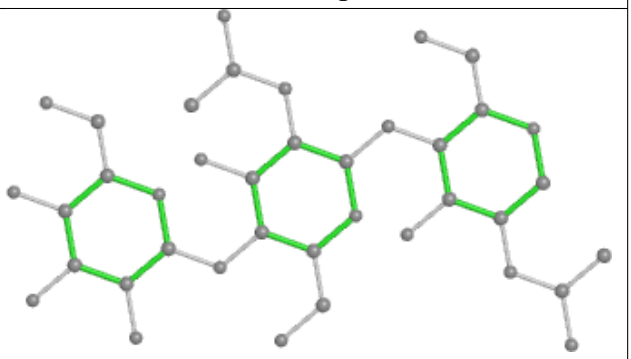
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

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	D	401	2	14,14,15	0.72	0	17,19,21	1.17	1 (5%)
5	NAG	E	330	1	14,14,15	0.91	1 (7%)	17,19,21	1.00	0
4	SIA	E	329	-	18,21,21	1.19	1 (5%)	21,31,31	1.21	1 (4%)
5	NAG	E	334	1	14,14,15	0.91	0	17,19,21	1.41	1 (5%)
4	SIA	A	329	-	18,21,21	1.21	1 (5%)	21,31,31	1.27	2 (9%)
5	NAG	F	401	2	14,14,15	0.70	0	17,19,21	1.12	1 (5%)
5	NAG	A	330	1	14,14,15	0.81	0	17,19,21	1.03	0
4	SIA	C	329	-	18,21,21	1.21	1 (5%)	21,31,31	1.36	3 (14%)
5	NAG	C	334	1	14,14,15	0.90	0	17,19,21	1.36	1 (5%)
5	NAG	C	330	1	14,14,15	0.75	0	17,19,21	1.13	1 (5%)
5	NAG	E	348	1	14,14,15	0.66	0	17,19,21	1.09	1 (5%)
5	NAG	C	348	1	14,14,15	0.69	0	17,19,21	1.04	1 (5%)
5	NAG	A	334	1	14,14,15	0.93	0	17,19,21	1.44	2 (11%)
5	NAG	A	348	1	14,14,15	0.80	1 (7%)	17,19,21	1.08	0
5	NAG	B	401	2	14,14,15	0.64	0	17,19,21	1.11	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	D	401	2	-	0/6/23/26	0/1/1/1
5	NAG	E	330	1	-	0/6/23/26	0/1/1/1
4	SIA	E	329	-	-	0/14/38/38	0/1/1/1
5	NAG	E	334	1	-	1/6/23/26	0/1/1/1
4	SIA	A	329	-	-	0/14/38/38	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
5	NAG	A	330	1	-	2/6/23/26	0/1/1/1
4	SIA	C	329	-	-	0/14/38/38	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	E	348	1	-	1/6/23/26	0/1/1/1
5	NAG	C	348	1	-	1/6/23/26	0/1/1/1
5	NAG	A	334	1	-	1/6/23/26	0/1/1/1
5	NAG	A	348	1	-	1/6/23/26	0/1/1/1
5	NAG	B	401	2	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	329	SIA	C3-C2	4.50	1.57	1.51
4	C	329	SIA	C3-C2	4.47	1.57	1.51
4	A	329	SIA	C3-C2	4.40	1.56	1.51
5	E	330	NAG	C4-C5	2.52	1.58	1.53
5	A	348	NAG	C1-C2	2.17	1.55	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	334	NAG	C1-O5-C5	3.48	116.91	112.19
5	E	334	NAG	C1-O5-C5	3.33	116.71	112.19
5	D	401	NAG	C1-O5-C5	3.28	116.63	112.19
5	B	401	NAG	C1-O5-C5	3.12	116.42	112.19
5	C	334	NAG	C1-O5-C5	3.11	116.40	112.19
5	F	401	NAG	C1-O5-C5	2.90	116.12	112.19
4	C	329	SIA	O8-C8-C7	2.44	115.03	109.10
4	C	329	SIA	C8-C7-C6	-2.40	108.48	113.03
4	C	329	SIA	C11-C10-N5	2.33	120.04	116.10
4	A	329	SIA	C8-C7-C6	-2.26	108.75	113.03
4	E	329	SIA	C8-C7-C6	-2.17	108.91	113.03
5	C	330	NAG	C8-C7-N2	2.13	119.71	116.10
4	A	329	SIA	C11-C10-N5	2.08	119.61	116.10
5	C	348	NAG	C8-C7-N2	2.05	119.58	116.10
5	E	348	NAG	C8-C7-N2	2.03	119.54	116.10
5	A	334	NAG	C1-C2-N2	2.01	113.92	110.49

There are no chirality outliers.

All (8) 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

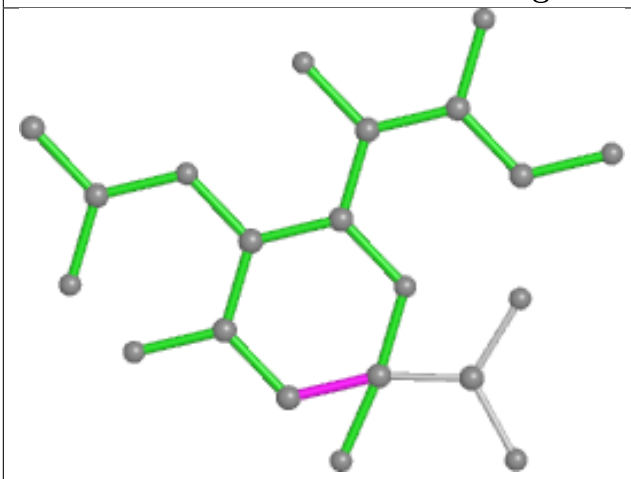
There are no ring outliers.

3 monomers are involved in 3 short contacts:

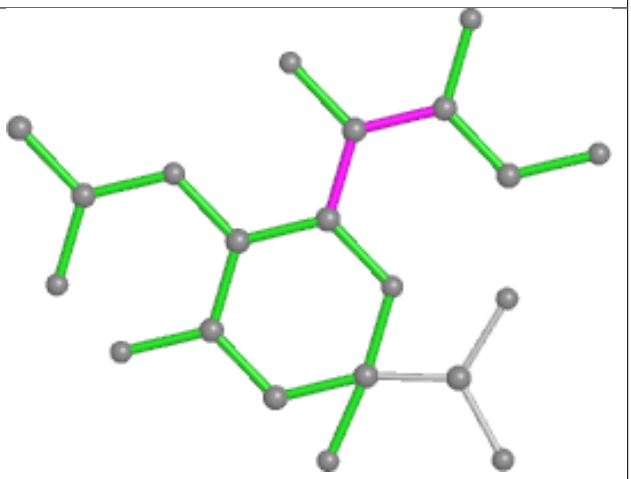
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	329	SIA	1	0
4	A	329	SIA	1	0
4	C	329	SIA	1	0

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 then 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.

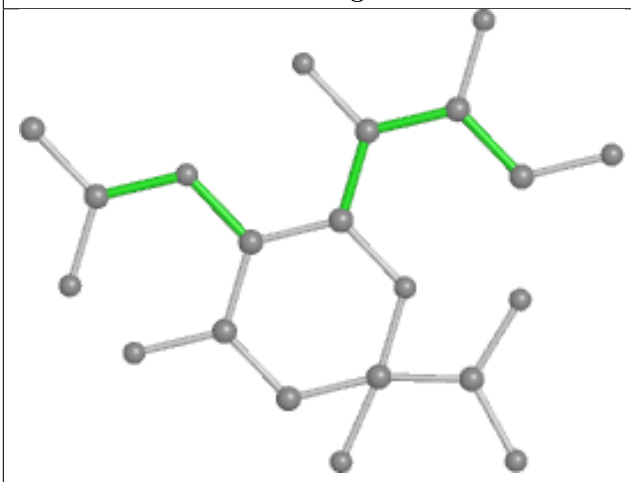
Ligand SIA E 329



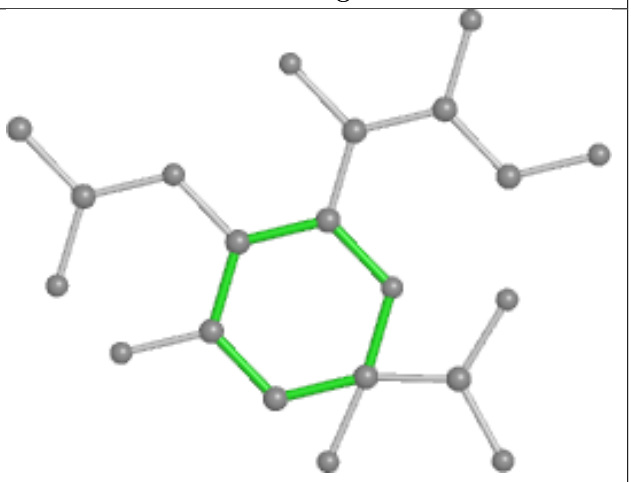
Bond lengths



Bond angles

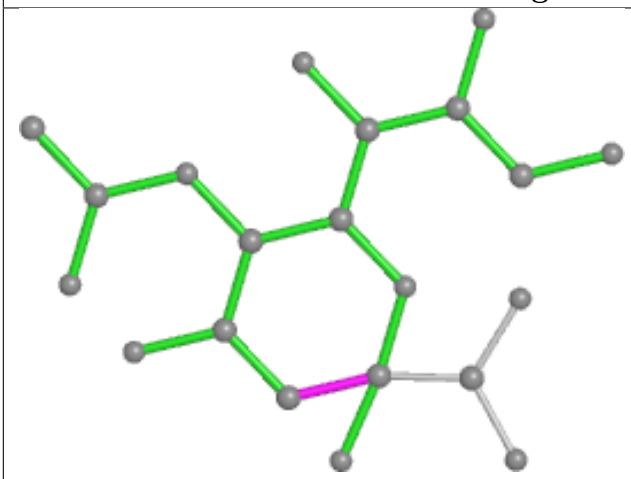


Torsions

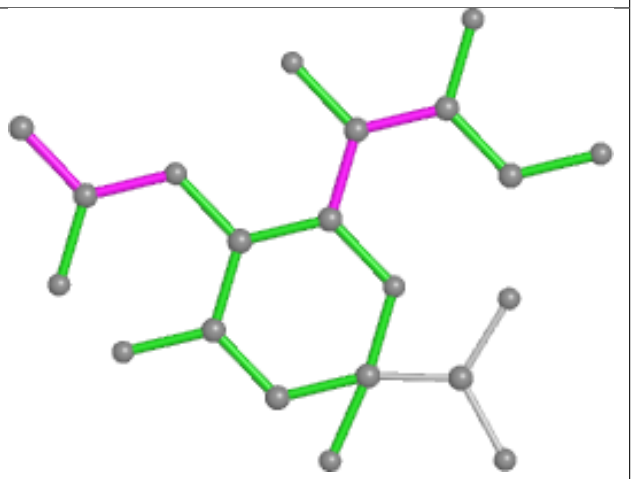


Rings

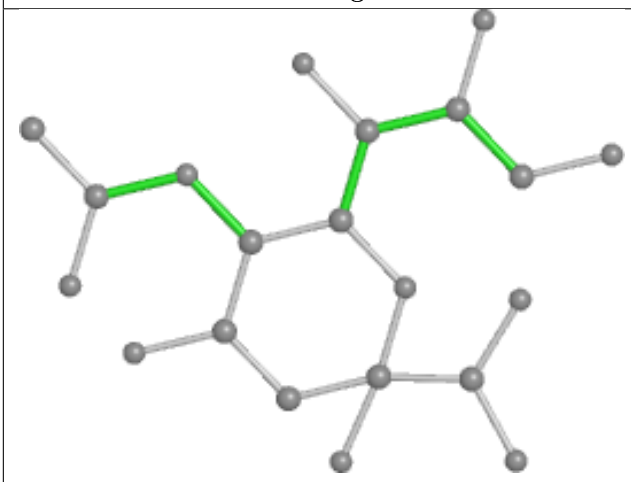
Ligand SIA A 329



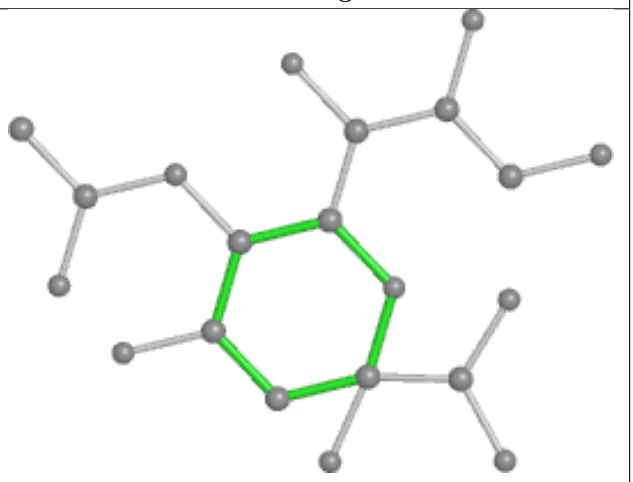
Bond lengths



Bond angles

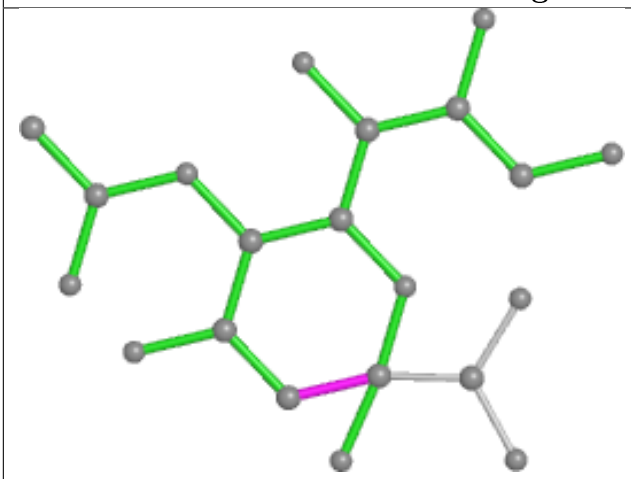


Torsions

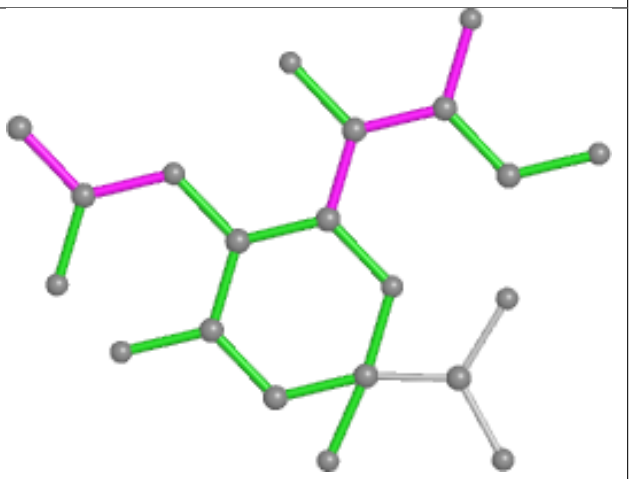


Rings

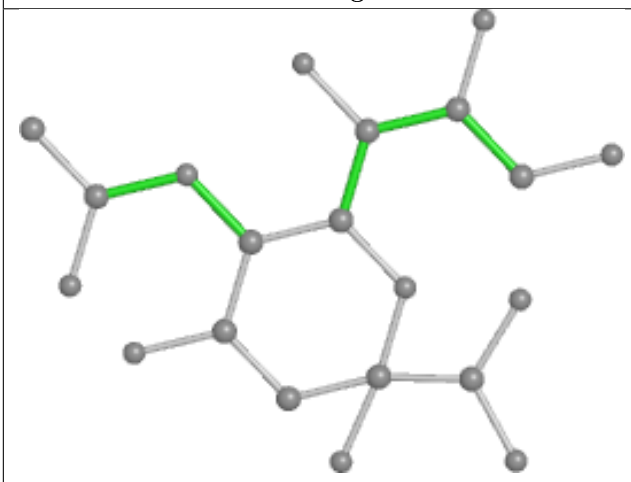
Ligand SIA C 329



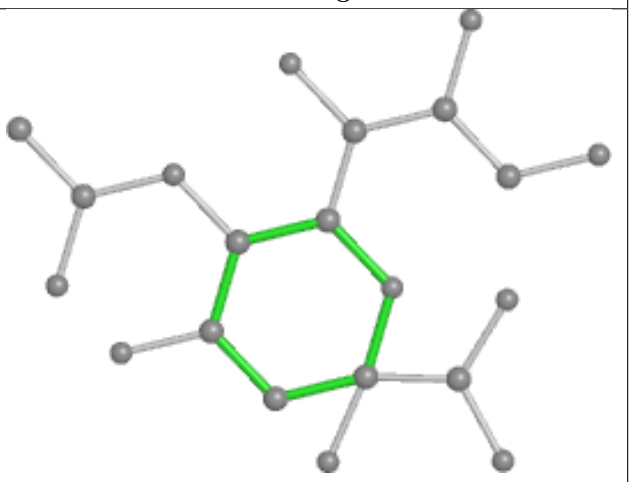
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.84	6 (1%)	68	55	3, 22, 51, 133	0
1	C	328/328 (100%)	-0.85	8 (2%)	59	44	2, 21, 47, 129	0
1	E	328/328 (100%)	-0.91	7 (2%)	63	49	3, 21, 46, 131	0
2	B	175/175 (100%)	-0.91	1 (0%)	89	83	2, 16, 47, 98	0
2	D	175/175 (100%)	-0.99	1 (0%)	89	83	2, 15, 46, 99	0
2	F	175/175 (100%)	-0.97	1 (0%)	89	83	2, 15, 46, 98	0
All	All	1509/1509 (100%)	-0.90	24 (1%)	72	59	2, 20, 50, 133	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	GLY	7.9
1	E	2	ASP	7.4
1	A	6	ASN	5.6
2	D	175	GLY	5.0
1	A	8	ASN	4.9
1	C	5	GLY	4.8
1	E	5	GLY	4.3
2	F	175	GLY	4.3
2	B	175	GLY	3.8
1	A	4	PRO	3.6
1	C	6	ASN	3.2
1	C	2	ASP	3.2
1	A	1	GLN	3.2
1	C	4	PRO	3.2
1	C	8	ASN	3.0
1	E	4	PRO	3.0
1	A	2	ASP	2.7
1	E	328	THR	2.6
1	C	1	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	1	GLN	2.3
1	E	3	LEU	2.3
1	C	328	THR	2.3
1	C	3	LEU	2.2
1	E	6	ASN	2.1

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)

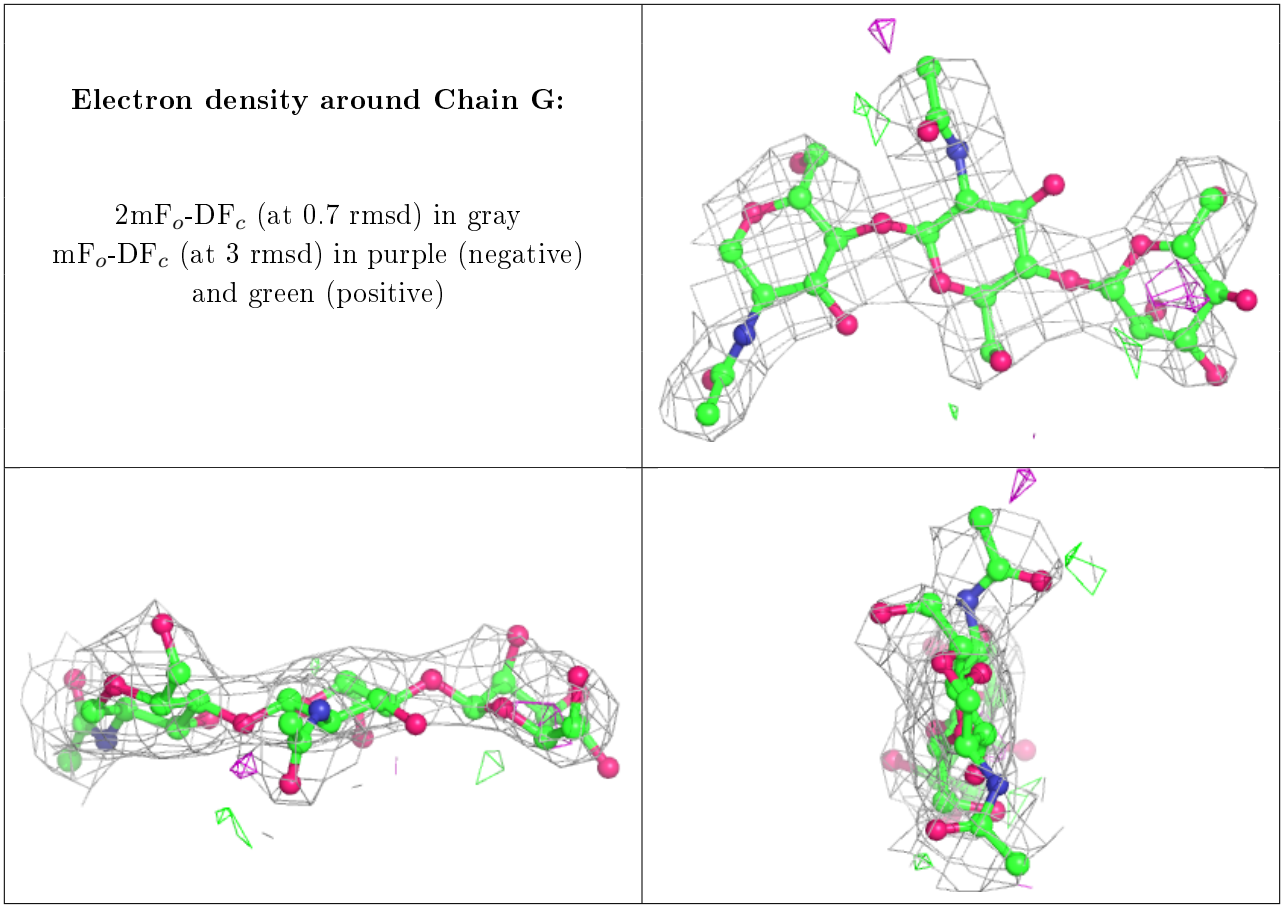
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	I	3	11/12	0.83	0.29	59,61,63,64	0
3	MAN	H	3	11/12	0.86	0.32	60,62,64,65	0
3	NAG	H	1	14/15	0.88	0.21	38,42,44,45	0
3	MAN	G	3	11/12	0.88	0.26	57,59,60,60	0
3	NAG	H	2	14/15	0.90	0.22	48,50,54,56	0
3	NAG	G	2	14/15	0.92	0.21	48,51,54,54	0
3	NAG	I	2	14/15	0.92	0.19	48,51,53,55	0
3	NAG	G	1	14/15	0.94	0.17	38,41,43,45	0
3	NAG	I	1	14/15	0.97	0.12	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.

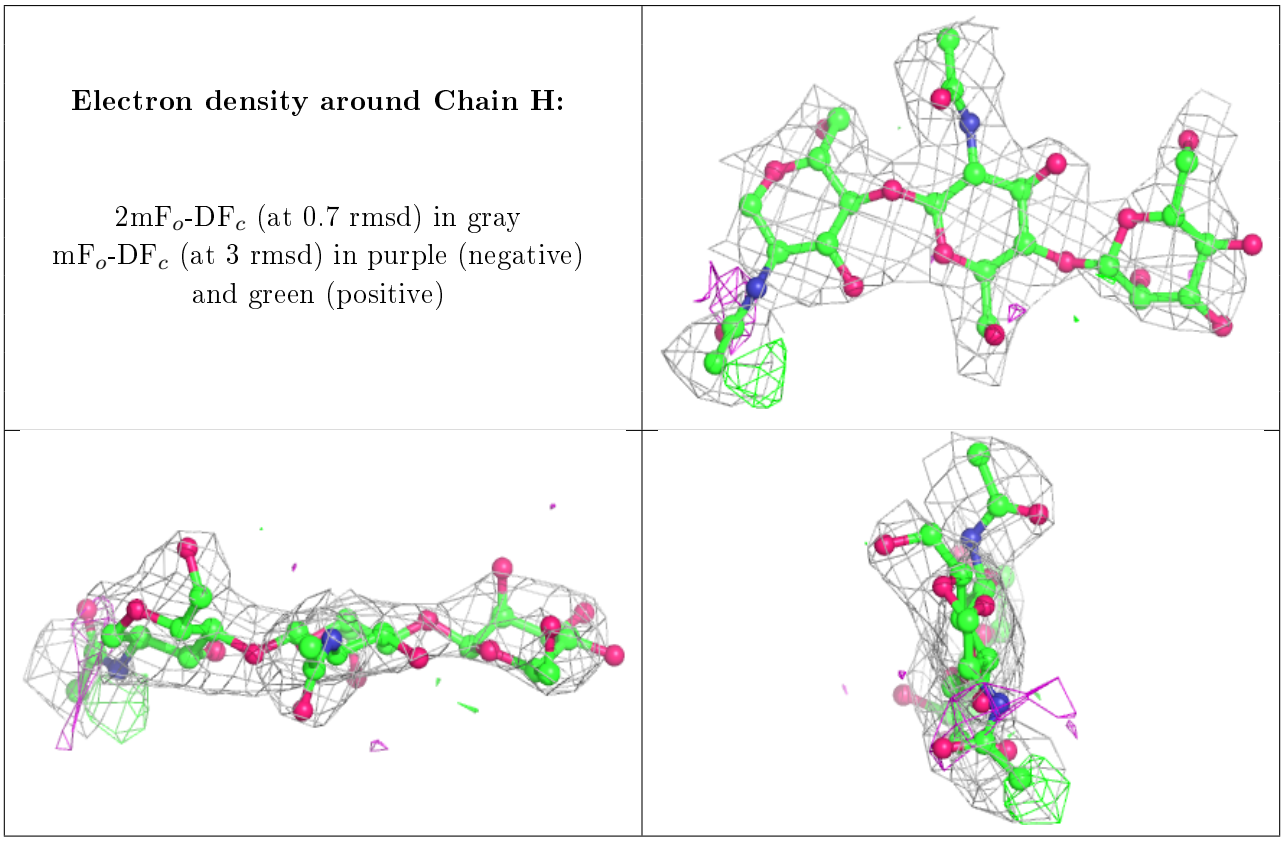
Electron density around Chain G:

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



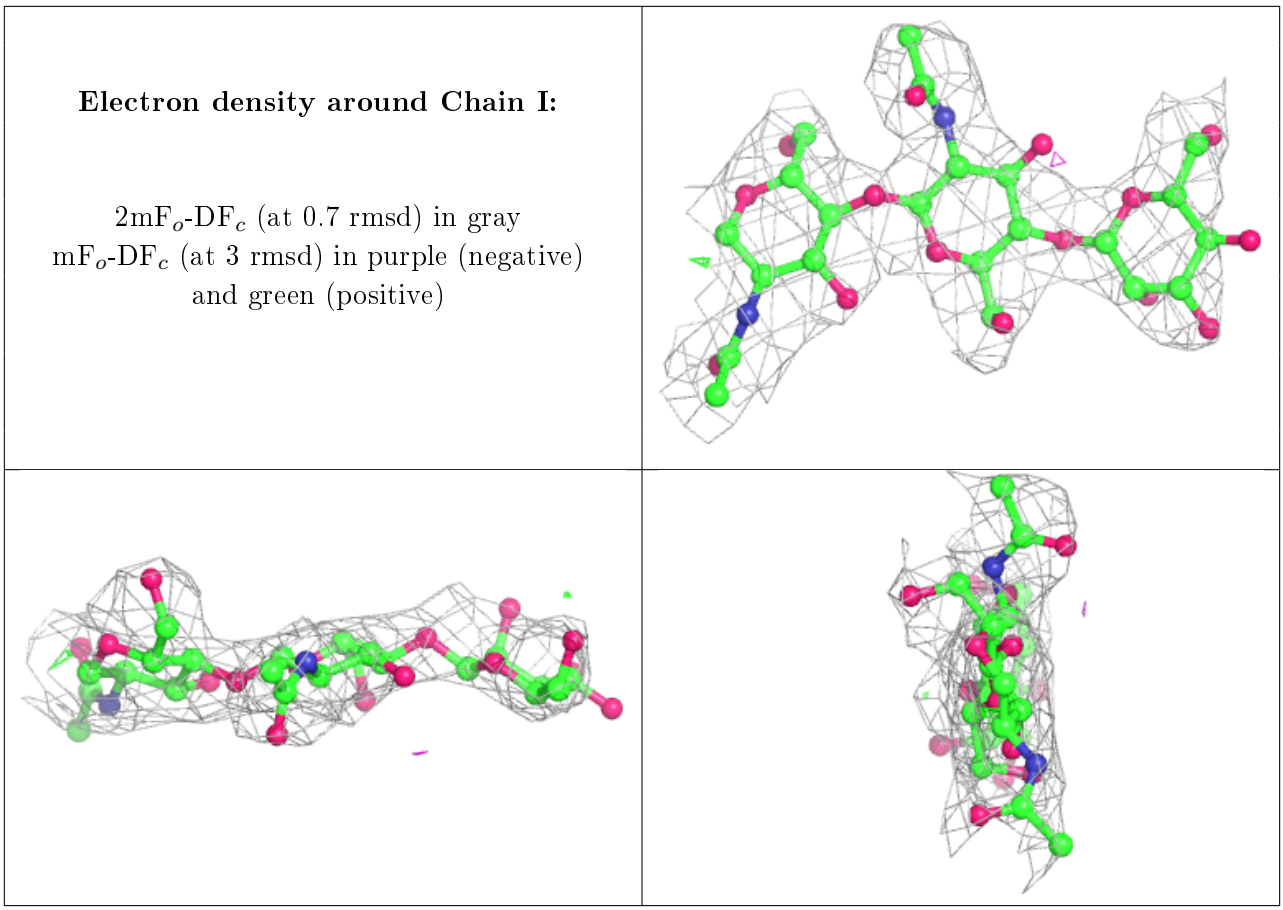
Electron density around Chain H:

$2mF_o$-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, 95^{th} 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
4	SIA	C	329	21/21	0.80	0.35	49,50,50,50	21
4	SIA	A	329	21/21	0.83	0.30	49,49,50,50	21
5	NAG	F	401	14/15	0.84	0.31	50,54,56,56	0
4	SIA	E	329	21/21	0.86	0.28	49,49,50,50	21
5	NAG	E	348	14/15	0.86	0.27	36,40,42,42	0
5	NAG	D	401	14/15	0.87	0.28	51,55,56,57	0
5	NAG	A	334	14/15	0.88	0.22	37,41,42,43	0
5	NAG	E	334	14/15	0.89	0.20	38,40,43,44	0
5	NAG	A	348	14/15	0.89	0.20	34,39,40,40	0
5	NAG	E	330	14/15	0.90	0.25	39,43,44,44	0
5	NAG	A	330	14/15	0.90	0.26	38,42,44,44	0
5	NAG	B	401	14/15	0.90	0.23	51,54,56,56	0
5	NAG	C	334	14/15	0.92	0.19	38,41,42,43	0

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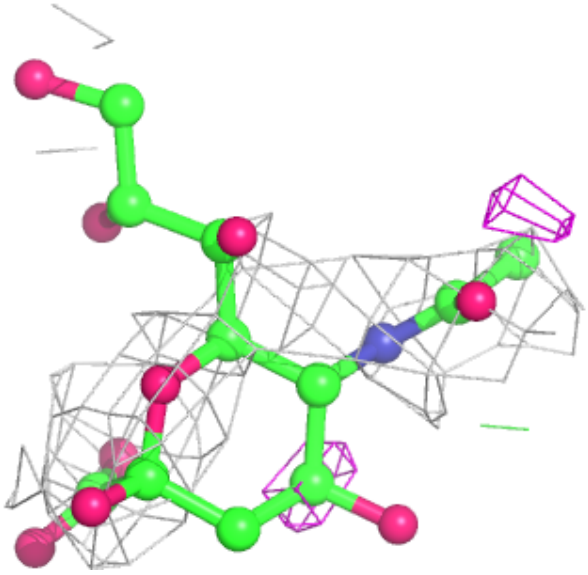
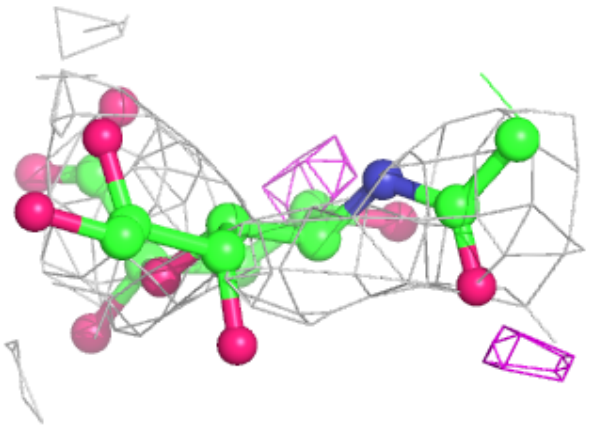
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	C	348	14/15	0.93	0.20	35,39,41,42	0
5	NAG	C	330	14/15	0.94	0.18	38,41,43,43	0

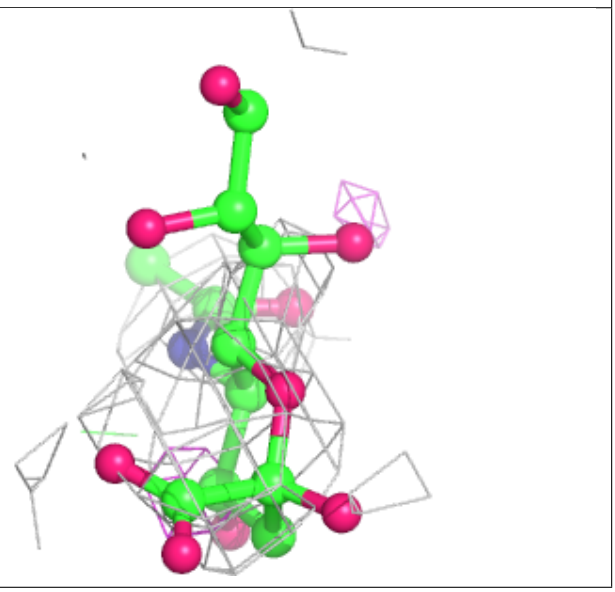
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SIA 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)

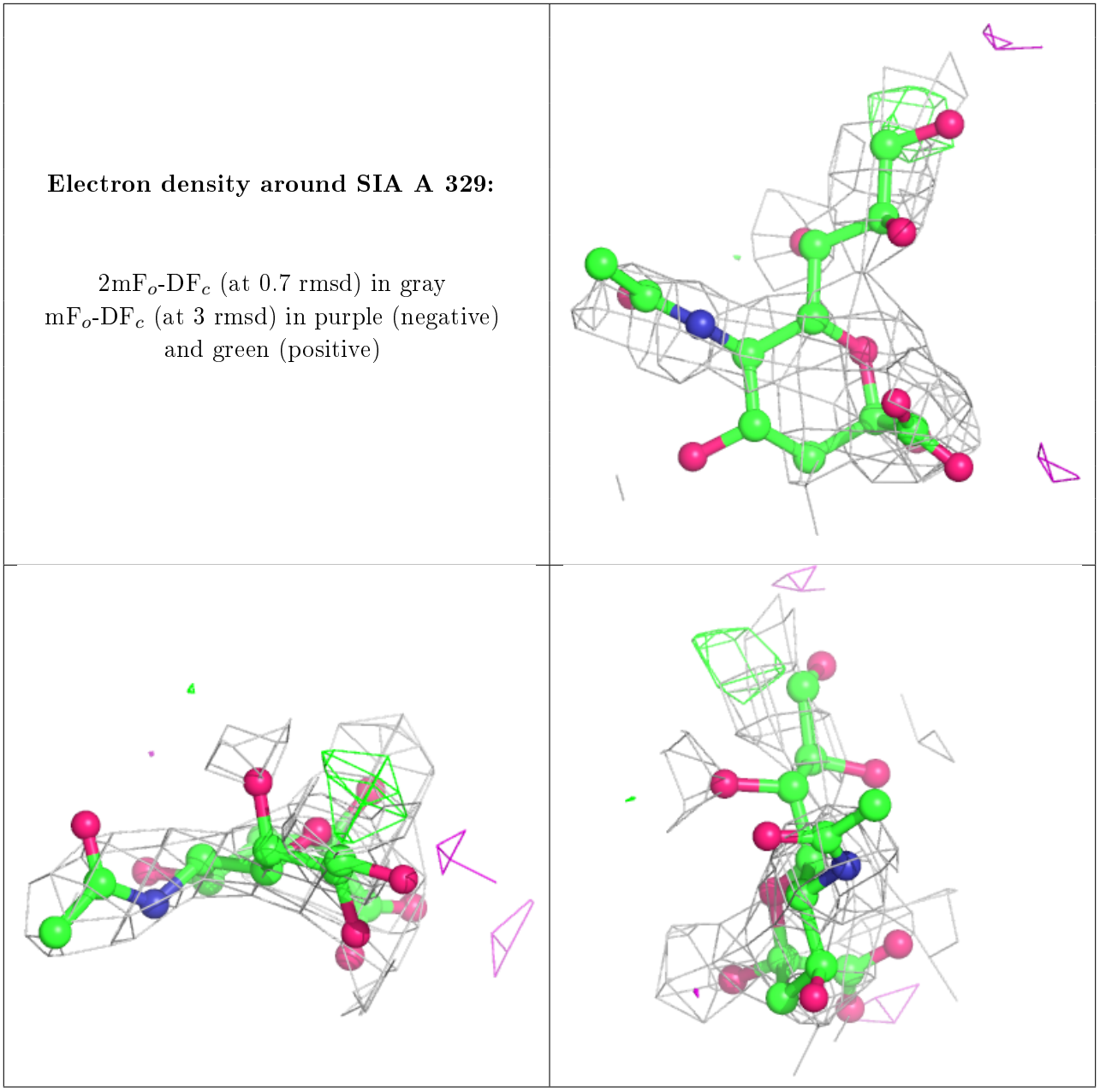






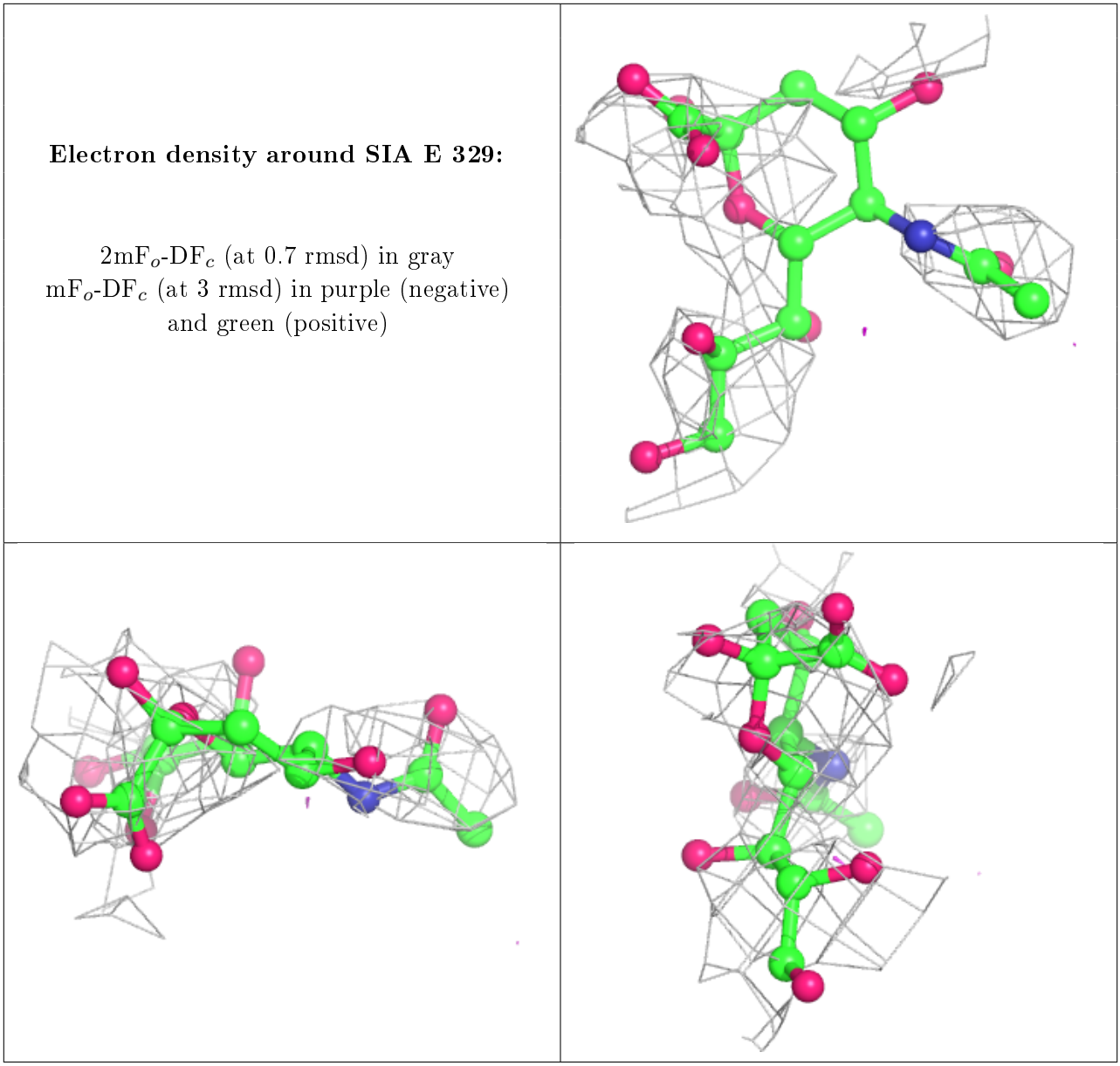
Electron density around SIA A 329:

$2mF_o$-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 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

There are no such residues in this entry.