



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:44 AM UTC

PDB ID : 9GBQ / pdb_00009gbq
Title : Human Angiotensin-1 converting enzyme N-domain in complex with a diprolyl inhibitor- SG15
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Deposited on : 2024-07-31
Resolution : 1.90 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

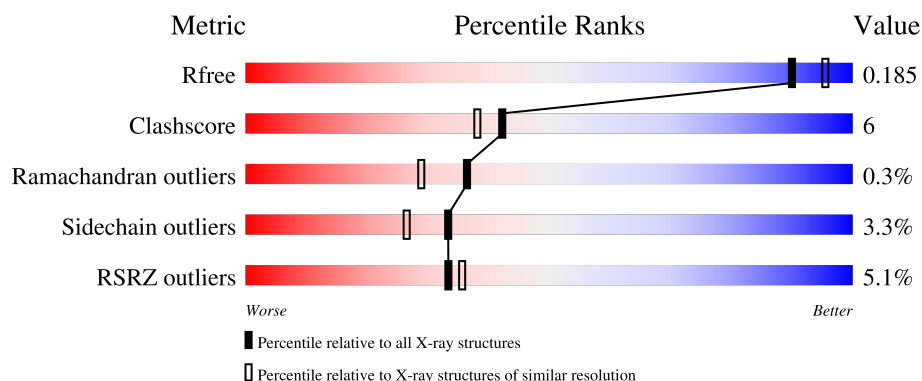
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	628	4% 75% 18% ..
1	B	628	6% 77% 16% .
2	D	2	100%
3	F	4	100%
4	G	3	100%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 10703 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 Angiotensin-converting enzyme, soluble form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	604	Total	C	N	O	S	0	0	0
			4935	3171	847	898	19			
1	B	602	Total	C	N	O	S	0	0	0
			4916	3159	842	896	19			

There are 16 discrepancies between the modelled and reference sequences:

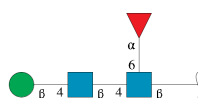
Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	engineered mutation	UNP P12821
A	25	GLN	ASN	engineered mutation	UNP P12821
A	82	GLN	ASN	engineered mutation	UNP P12821
A	117	GLN	ASN	engineered mutation	UNP P12821
A	131	GLN	ASN	engineered mutation	UNP P12821
A	289	GLN	ASN	engineered mutation	UNP P12821
A	545	ARG	GLN	engineered mutation	UNP P12821
A	576	LEU	PRO	engineered mutation	UNP P12821
B	9	GLN	ASN	engineered mutation	UNP P12821
B	25	GLN	ASN	engineered mutation	UNP P12821
B	82	GLN	ASN	engineered mutation	UNP P12821
B	117	GLN	ASN	engineered mutation	UNP P12821
B	131	GLN	ASN	engineered mutation	UNP P12821
B	289	GLN	ASN	engineered mutation	UNP P12821
B	545	ARG	GLN	engineered mutation	UNP P12821
B	576	LEU	PRO	engineered mutation	UNP P12821

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



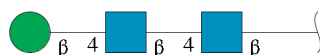
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



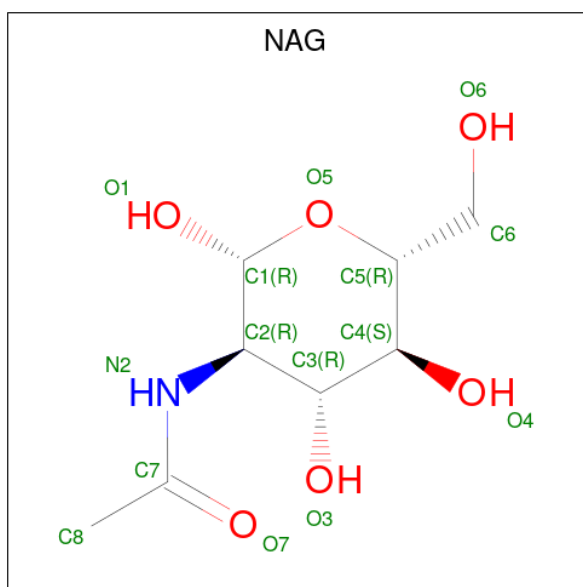
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	4	Total	C	N	O	0	0	0
			49	28	2	19			

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



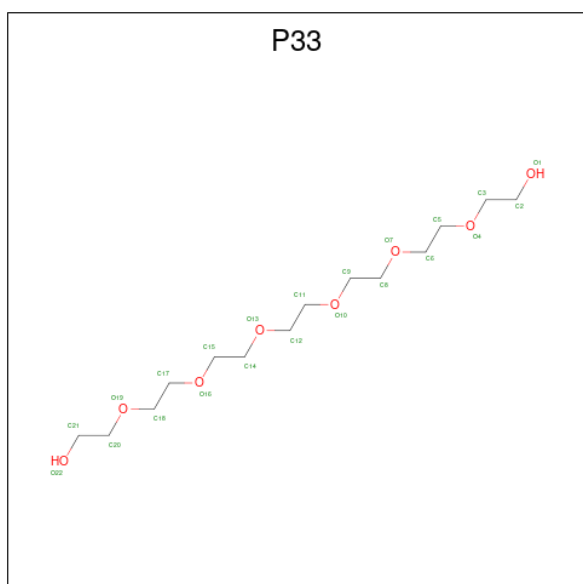
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



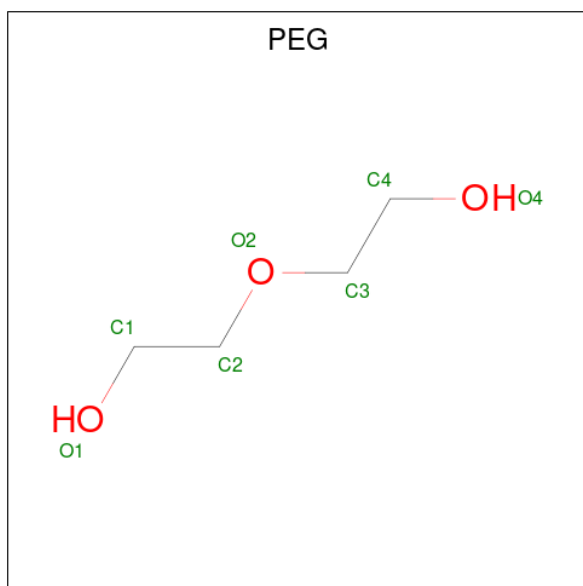
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is 3,6,9,12,15,18-HEXAOSAICOSANE-1,20-DIOL (CCD ID: P33) (formula: $C_{14}H_{30}O_8$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			22	14	8		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		
7	A	1	Total	C	O	0	0
			7	4	3		
7	A	1	Total	C	O	0	0
			7	4	3		
7	B	1	Total	C	O	0	0
			7	4	3		

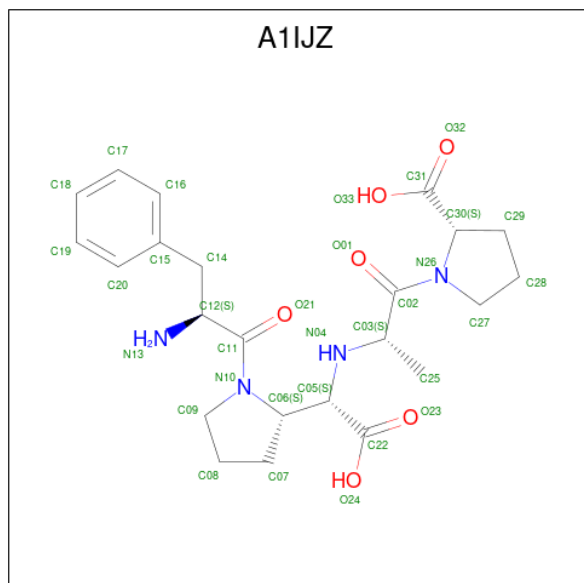
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Zn	0	0
			1	1		
8	B	1	Total	Zn	0	0
			1	1		

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

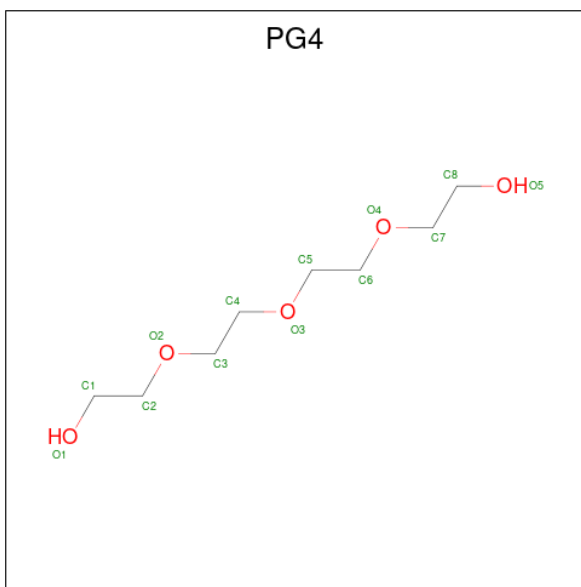
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Cl 1 1	0	0
9	B	1	Total Cl 1 1	0	0

- Molecule 10 is (2S)-1-[(2S)-2-[[[(1S)-1-[(2S)-1-[(2S)-2-azanyl-3-phenyl-propanoyl]pyrrolidin-2-yl]-2-oxidanyl-2-oxidanylidene-ethyl]amino]propanoyl]pyrrolidine-2-carboxylic acid (CCD ID: A1IJZ) (formula: C₂₃H₃₂N₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C N O 33 23 4 6	0	0
10	B	1	Total C N O 33 23 4 6	0	0

- Molecule 11 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	B	1	Total	Mg	0	0
			1	1		

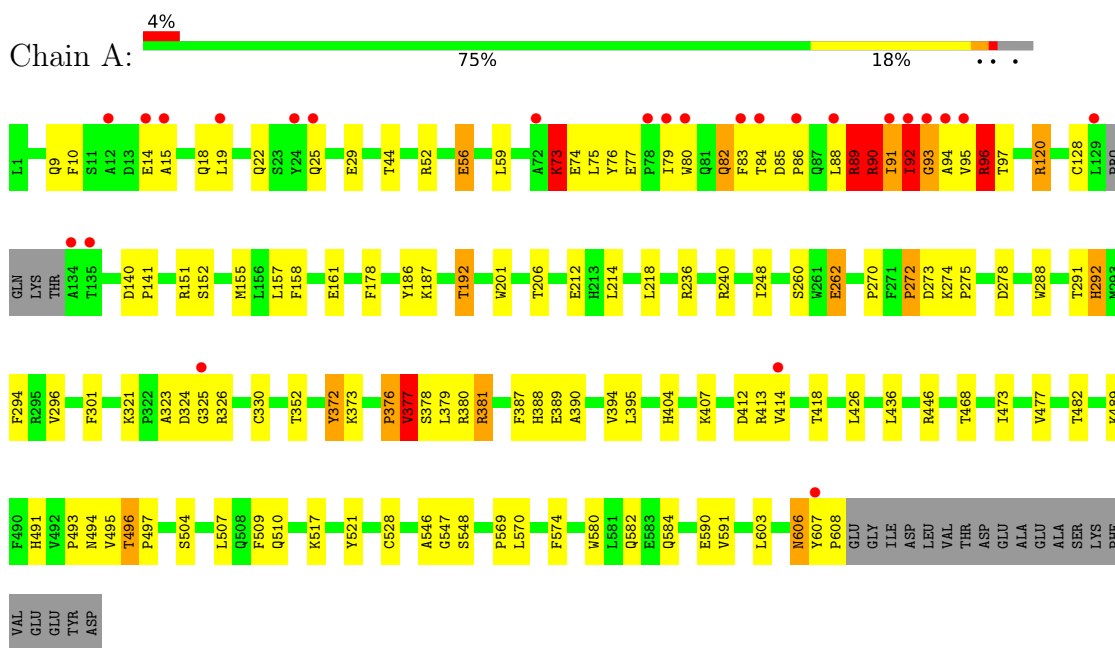
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	327	Total	O	0	0
			327	327		
13	B	237	Total	O	0	0
			237	237		

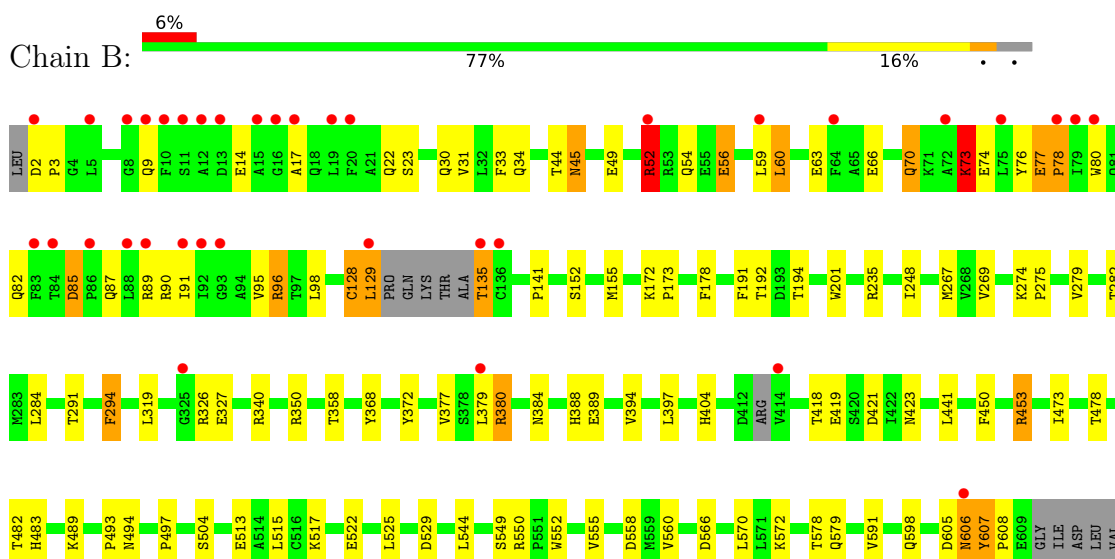
3 Residue-property plots

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

- Molecule 1: Angiotensin-converting enzyme, soluble form



- Molecule 1: Angiotensin-converting enzyme, soluble form



THR
ASP
GLU
ALA
GLU
ALA
SER
LYS
PHE
VAL
GLU
TYR
ASP

- Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  100%

MAG1
FUC2

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

MAG1
MAG2
BMA3
FUC4

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

Chain G:  100%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.49Å 77.17Å 81.44Å 88.55° 64.52° 75.14°	Depositor
Resolution (Å)	73.28 – 1.90 73.28 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.8 (73.28-1.90) 96.0 (73.28-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.177 , 0.212 0.180 , 0.185	Depositor DCC
R_{free} test set	5769 reflections (4.06%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10703	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, BMA, P33, A1IJZ, MG, PEG, ZN, CL, PG4, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.80	1/5090 (0.0%)	1.47	62/6933 (0.9%)
1	B	0.71	0/5070	1.41	55/6905 (0.8%)
All	All	0.76	1/10160 (0.0%)	1.44	117/13838 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	3
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	381	ARG	NE-CZ	5.78	1.39	1.33

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	54	GLN	CB-CA-C	10.32	128.40	110.85
1	B	54	GLN	N-CA-CB	-10.06	95.28	110.16
1	A	507	LEU	N-CA-CB	-9.61	95.39	110.28
1	B	56	GLU	CB-CG-CD	8.96	127.84	112.60
1	A	96	ARG	CB-CA-C	8.75	127.25	110.27
1	B	606	ASN	CB-CA-C	8.60	125.67	111.23
1	A	85	ASP	CB-CA-C	8.56	127.03	110.17
1	A	509	PHE	CA-CB-CG	-8.18	105.62	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	178	PHE	CA-CB-CG	-7.87	105.94	113.80
1	B	279	VAL	N-CA-C	-7.76	105.00	112.29
1	B	578	THR	CA-CB-OG1	-7.67	98.10	109.60
1	A	387	PHE	N-CA-CB	7.65	121.36	110.12
1	A	496	THR	CA-CB-OG1	7.64	121.07	109.60
1	B	482	THR	CA-CB-OG1	-7.57	98.25	109.60
1	B	129	LEU	N-CA-CB	7.48	123.22	110.50
1	A	214	LEU	N-CA-CB	7.44	120.80	110.01
1	A	96	ARG	CG-CD-NE	-7.28	95.99	112.00
1	A	151	ARG	CD-NE-CZ	7.24	134.54	124.40
1	A	85	ASP	CA-CB-CG	7.21	119.81	112.60
1	B	52	ARG	N-CA-CB	7.16	120.39	110.01
1	A	413	ARG	N-CA-CB	-7.14	98.78	110.43
1	B	453	ARG	CB-CG-CD	7.04	127.49	111.30
1	A	387	PHE	CB-CA-C	-6.88	99.38	110.79
1	A	44	THR	CA-CB-OG1	-6.87	99.30	109.60
1	A	292	HIS	CA-CB-CG	-6.84	106.96	113.80
1	A	206	THR	CA-CB-OG1	-6.81	99.39	109.60
1	B	483	HIS	CA-CB-CG	-6.75	107.05	113.80
1	B	566	ASP	CA-CB-CG	6.71	119.31	112.60
1	A	29	GLU	CB-CA-C	6.60	121.75	110.79
1	A	151	ARG	NE-CZ-NH2	6.51	125.06	119.20
1	A	192	THR	CA-CB-OG1	-6.50	99.84	109.60
1	A	404	HIS	CA-CB-CG	-6.47	107.33	113.80
1	B	52	ARG	CA-CB-CG	6.46	127.02	114.10
1	A	418	THR	CA-CB-OG1	-6.44	99.93	109.60
1	A	291	THR	CA-CB-OG1	-6.35	100.07	109.60
1	A	494	ASN	CA-CB-CG	-6.29	106.31	112.60
1	B	418	THR	CB-CA-C	6.29	121.80	109.72
1	A	128	CYS	CB-CA-C	6.29	120.12	109.50
1	B	478	THR	CA-CB-OG1	-6.28	100.18	109.60
1	B	128	CYS	CB-CA-C	6.25	122.60	109.79
1	B	73	LYS	CB-CG-CD	6.24	125.65	111.30
1	B	282	THR	CA-CB-OG1	-6.16	100.36	109.60
1	B	85	ASP	CA-CB-CG	6.11	118.71	112.60
1	A	10	PHE	N-CA-CB	-6.06	100.25	111.52
1	A	377	VAL	N-CA-CB	6.04	118.02	110.47
1	A	590	GLU	CB-CG-CD	6.00	122.81	112.60
1	A	606	ASN	CA-CB-CG	-5.99	106.61	112.60
1	B	77	GLU	CB-CG-CD	5.98	122.77	112.60
1	B	22	GLN	CA-C-N	5.94	128.24	120.28
1	B	22	GLN	C-N-CA	5.94	128.24	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412	ASP	CB-CA-C	-5.92	101.54	110.90
1	A	151	ARG	NE-CZ-NH1	-5.88	115.62	121.50
1	B	607	TYR	CB-CA-C	5.79	117.24	109.42
1	B	591	VAL	N-CA-CB	-5.78	104.41	111.00
1	A	272	PRO	N-CA-C	5.74	121.31	113.84
1	A	161	GLU	CB-CG-CD	5.72	122.32	112.60
1	A	186	TYR	CA-CB-CG	-5.72	103.61	113.90
1	B	96	ARG	N-CA-CB	-5.67	100.45	110.42
1	B	73	LYS	CB-CA-C	5.66	119.77	110.88
1	B	85	ASP	CB-CA-C	5.66	118.96	109.85
1	B	606	ASN	CA-CB-CG	5.65	118.25	112.60
1	A	381	ARG	CB-CG-CD	5.64	124.28	111.30
1	B	419	GLU	CB-CA-C	-5.63	101.28	110.85
1	B	380	ARG	N-CA-CB	5.63	117.54	110.45
1	A	373	LYS	CD-CE-NZ	-5.59	94.02	111.90
1	A	574	PHE	N-CA-CB	5.58	118.98	110.44
1	B	135	THR	CA-CB-OG1	-5.57	101.24	109.60
1	A	446	ARG	CA-CB-CG	5.56	125.22	114.10
1	B	235	ARG	CG-CD-NE	5.56	124.23	112.00
1	A	178	PHE	CA-CB-CG	-5.55	108.25	113.80
1	A	56	GLU	CB-CG-CD	5.53	122.00	112.60
1	B	70	GLN	CB-CA-C	-5.51	102.00	110.81
1	B	579	GLN	N-CA-CB	-5.50	102.10	110.07
1	B	49	GLU	CB-CA-C	5.49	119.91	110.79
1	B	192	THR	CA-CB-OG1	-5.47	101.40	109.60
1	B	423	ASN	CA-CB-CG	5.46	118.06	112.60
1	B	377	VAL	N-CA-CB	5.46	117.29	110.47
1	B	560	VAL	N-CA-CB	5.46	118.21	112.21
1	B	9	GLN	CB-CA-C	5.44	119.17	109.38
1	B	404	HIS	CA-CB-CG	-5.43	108.37	113.80
1	A	482	THR	CA-CB-OG1	-5.42	101.47	109.60
1	B	60	LEU	N-CA-CB	-5.40	102.18	110.01
1	A	294	PHE	CA-CB-CG	-5.39	108.41	113.80
1	A	278	ASP	CB-CA-C	5.34	119.63	110.81
1	A	372	TYR	CA-CB-CG	5.34	123.52	113.90
1	A	413	ARG	CA-CB-CG	5.32	124.73	114.10
1	B	191	PHE	CA-CB-CG	-5.29	108.51	113.80
1	A	407	LYS	N-CA-CB	5.29	118.36	110.22
1	A	91	ILE	N-CA-CB	5.28	116.37	110.51
1	A	93	GLY	CA-C-N	5.28	127.67	120.54
1	A	93	GLY	C-N-CA	5.28	127.67	120.54
1	B	494	ASN	CA-CB-CG	-5.28	107.32	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	419	GLU	N-CA-CB	5.27	117.96	110.16
1	B	49	GLU	N-CA-CB	5.26	117.85	110.12
1	A	92	ILE	CA-C-O	-5.25	114.22	120.78
1	B	33	PHE	N-CA-CB	5.24	117.79	109.82
1	B	605	ASP	CA-C-N	-5.24	115.22	123.13
1	B	605	ASP	C-N-CA	-5.24	115.22	123.13
1	A	90	ARG	CB-CG-CD	5.23	123.33	111.30
1	A	468	THR	CA-CB-OG1	-5.20	101.80	109.60
1	A	74	GLU	N-CA-CB	-5.19	102.48	110.16
1	A	582	GLN	CB-CA-C	-5.18	102.04	110.85
1	A	82	GLN	CB-CA-C	5.18	119.49	110.94
1	A	73	LYS	CB-CA-C	5.18	120.61	110.67
1	B	294	PHE	CA-CB-CG	-5.17	108.63	113.80
1	A	496	THR	CB-CA-C	5.16	116.39	109.42
1	A	491	HIS	CA-CB-CG	-5.16	108.64	113.80
1	A	591	VAL	N-CA-CB	-5.14	104.82	110.99
1	B	529	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	14	GLU	CB-CG-CD	5.12	121.30	112.60
1	B	291	THR	CA-CB-OG1	-5.11	101.94	109.60
1	A	236	ARG	CD-NE-CZ	5.09	131.52	124.40
1	A	352	THR	CA-CB-CG2	5.08	119.13	110.50
1	B	358	THR	CA-CB-OG1	-5.08	101.98	109.60
1	A	89	ARG	CB-CA-C	5.07	120.52	110.42
1	A	377	VAL	CB-CA-C	-5.07	105.40	112.04
1	B	380	ARG	CB-CA-C	-5.04	104.77	111.88

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	ARG	Sidechain
1	A	240	ARG	Sidechain
1	A	380	ARG	Sidechain
1	A	89	ARG	Sidechain
1	A	96	ARG	Sidechain
1	B	380	ARG	Sidechain
1	B	78	PRO	Peptide
1	B	90	ARG	Sidechain

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	4935	0	4717	71	0
1	B	4916	0	4686	48	0
2	D	24	0	22	0	0
3	F	49	0	43	0	0
4	G	39	0	34	2	0
5	A	28	0	26	0	0
5	B	14	0	13	0	0
6	A	22	0	30	3	0
7	A	21	0	30	1	0
7	B	7	0	10	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	33	0	0	0	0
10	B	33	0	0	0	0
11	B	13	0	18	5	0
12	B	1	0	0	0	0
13	A	327	0	0	3	0
13	B	237	0	0	9	0
All	All	10703	0	9629	124	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 6.

All (124) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:GLN:O	1:A:22:GLN:HG3	1.54	1.07
1:A:15:ALA:O	1:A:19:LEU:HD13	1.81	0.80
1:B:77:GLU:OE1	1:B:96:ARG:HD2	1.84	0.76
1:B:91:ILE:O	1:B:95:VAL:HG23	1.87	0.75
1:A:25:GLN:NE2	1:A:376:PRO:HB3	2.02	0.74
1:A:157:LEU:HD11	1:A:477:VAL:HG13	1.69	0.74
1:A:260:SER:OG	1:A:262:GLU:OE1	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:LEU:O	1:B:63:GLU:HG3	1.91	0.70
1:A:260:SER:OG	1:A:262:GLU:CD	2.34	0.69
1:B:379:LEU:HD13	1:B:549:SER:HB3	1.74	0.69
1:B:522:GLU:OE2	4:G:3:BMA:H3	1.94	0.68
1:A:477:VAL:HG12	1:A:603:LEU:HD21	1.78	0.66
1:A:90:ARG:HG2	1:A:91:ILE:N	2.11	0.65
1:B:52:ARG:O	1:B:56:GLU:HG3	1.98	0.64
1:A:155:MET:HE3	1:A:158:PHE:HB3	1.81	0.62
1:A:18:GLN:O	1:A:22:GLN:CG	2.41	0.62
1:A:607:TYR:CD1	1:A:608:PRO:HA	2.35	0.61
11:B:702:PG4:H42	13:B:874:HOH:O	1.98	0.61
1:A:324:ASP:OD1	1:A:326:ARG:HB2	2.01	0.61
1:A:75:LEU:HB3	1:A:76:TYR:CE1	2.36	0.60
1:A:88:LEU:O	1:A:92:ILE:HB	2.01	0.60
1:A:94:ALA:O	1:A:97:THR:HB	2.02	0.60
1:A:270:PRO:HD3	1:A:426:LEU:CD2	2.32	0.60
1:B:550:ARG:NH2	1:B:558:ASP:OD2	2.33	0.59
1:A:80:TRP:HA	1:A:83:PHE:CD2	2.37	0.59
1:A:59:LEU:HD22	13:A:1031:HOH:O	2.02	0.59
1:A:84:THR:O	1:A:86:PRO:HD3	2.03	0.59
1:B:441:LEU:C	1:B:441:LEU:HD12	2.28	0.58
1:A:510:GLN:HG2	1:A:569:PRO:HG2	1.86	0.58
1:B:66:GLU:O	1:B:70:GLN:HG2	2.04	0.58
11:B:702:PG4:H72	13:B:835:HOH:O	2.04	0.58
1:B:31:VAL:O	1:B:34:GLN:HG3	2.03	0.58
1:A:292:HIS:CE1	6:A:702:P33:H82	2.38	0.57
13:A:847:HOH:O	11:B:702:PG4:H11	2.04	0.57
1:B:340:ARG:HH11	1:B:340:ARG:HG3	1.69	0.57
1:B:17:ALA:HB2	1:B:76:TYR:CE1	2.40	0.57
1:A:92:ILE:O	1:A:95:VAL:N	2.26	0.56
1:A:381:ARG:HG3	1:A:381:ARG:HH11	1.71	0.56
1:B:76:TYR:O	1:B:80:TRP:HD1	1.89	0.56
1:B:73:LYS:HA	1:B:77:GLU:HG2	1.88	0.55
11:B:702:PG4:C4	13:B:874:HOH:O	2.54	0.55
1:A:158:PHE:HA	1:A:607:TYR:OH	2.07	0.55
1:A:274:LYS:HB3	1:A:275:PRO:CD	2.38	0.53
1:B:389:GLU:HB2	1:B:504:SER:HB2	1.91	0.53
1:B:379:LEU:HD13	1:B:549:SER:CB	2.40	0.52
1:A:521:TYR:CE2	1:A:528:CYS:HB2	2.44	0.51
1:A:570:LEU:C	1:A:570:LEU:HD23	2.35	0.51
1:A:52:ARG:O	1:A:56:GLU:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:GLU:HA	1:B:525:LEU:HD11	1.93	0.51
1:A:270:PRO:HD3	1:A:426:LEU:HD23	1.93	0.51
1:A:212:GLU:OE2	1:B:453:ARG:NH1	2.44	0.50
1:B:201:TRP:HZ3	1:B:497:PRO:HG2	1.75	0.50
1:A:88:LEU:C	1:A:90:ARG:H	2.20	0.50
1:A:274:LYS:HB3	1:A:275:PRO:HD2	1.94	0.50
1:B:384:ASN:HD22	1:B:552:TRP:CG	2.30	0.49
1:B:284:LEU:HD23	13:B:945:HOH:O	2.12	0.49
1:B:80:TRP:O	1:B:89:ARG:HG3	2.12	0.48
1:A:218:LEU:HD13	1:A:436:LEU:HD13	1.95	0.48
1:A:187:LYS:HE2	1:A:192:THR:O	2.14	0.48
1:B:326:ARG:HG2	1:B:327:GLU:N	2.29	0.48
1:A:296:VAL:HG22	7:A:704:PEG:H42	1.96	0.47
1:B:570:LEU:C	1:B:570:LEU:HD23	2.39	0.47
1:A:521:TYR:CD2	1:A:528:CYS:HB2	2.49	0.47
1:A:25:GLN:NE2	1:A:376:PRO:CB	2.75	0.47
1:A:83:PHE:O	1:A:89:ARG:NE	2.46	0.47
1:B:489:LYS:O	1:B:493:PRO:HD2	2.15	0.47
1:A:292:HIS:NE2	6:A:702:P33:H111	2.31	0.46
1:A:76:TYR:O	1:A:77:GLU:C	2.59	0.46
1:A:90:ARG:HG2	1:A:91:ILE:H	1.80	0.46
1:B:59:LEU:HG	13:B:943:HOH:O	2.15	0.46
1:B:155:MET:HE3	1:B:155:MET:HA	1.98	0.45
4:G:1:NAG:H62	4:G:2:NAG:H82	1.99	0.45
1:A:19:LEU:CD1	1:A:19:LEU:N	2.80	0.45
1:A:389:GLU:HB2	1:A:504:SER:HB2	1.98	0.45
1:B:274:LYS:HB3	1:B:275:PRO:HD2	1.99	0.45
1:B:2:ASP:OD1	1:B:3:PRO:HD2	2.17	0.45
1:B:201:TRP:CZ3	1:B:497:PRO:HG2	2.51	0.45
1:A:73:LYS:HD2	1:A:96:ARG:O	2.16	0.45
1:B:572:LYS:HE2	13:B:1006:HOH:O	2.16	0.45
1:B:194:THR:HB	1:B:450:PHE:CD1	2.51	0.44
1:A:88:LEU:C	1:A:90:ARG:N	2.75	0.44
1:A:75:LEU:C	1:A:76:TYR:CD1	2.96	0.44
1:A:187:LYS:HE3	1:A:187:LYS:HB2	1.34	0.44
1:A:201:TRP:CZ3	1:A:497:PRO:HG2	2.53	0.44
1:B:555:VAL:HG21	13:B:918:HOH:O	2.17	0.44
1:A:140:ASP:HA	1:A:141:PRO:HA	1.80	0.44
1:B:141:PRO:HB3	1:B:350:ARG:HD3	1.99	0.44
1:A:274:LYS:HA	1:A:274:LYS:HD3	1.82	0.44
1:B:267:MET:HE1	13:B:846:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:TYR:HA	1:B:608:PRO:HA	1.59	0.44
1:A:489:LYS:O	1:A:493:PRO:HD2	2.19	0.43
1:A:607:TYR:CG	1:A:608:PRO:HA	2.53	0.43
1:A:120:ARG:HB2	13:A:1003:HOH:O	2.17	0.42
1:A:323:ALA:C	1:A:325:GLY:H	2.26	0.42
1:B:294:PHE:CZ	1:B:319:LEU:HD22	2.53	0.42
1:B:129:LEU:HD23	1:B:129:LEU:HA	1.92	0.42
11:B:702:PG4:H61	13:B:813:HOH:O	2.19	0.42
1:A:495:VAL:HG12	1:A:495:VAL:O	2.20	0.42
1:B:44:THR:O	1:B:45:ASN:HB2	2.20	0.42
1:B:394:VAL:HG11	1:B:515:LEU:HD12	2.01	0.42
1:A:80:TRP:O	1:A:89:ARG:HD3	2.20	0.42
1:A:301:PHE:CZ	1:A:395:LEU:HD22	2.55	0.41
1:A:248:ILE:O	1:A:473:ILE:HA	2.19	0.41
1:A:288:TRP:CD1	6:A:702:P33:H52	2.54	0.41
1:A:379:LEU:HA	1:A:548:SER:OG	2.20	0.41
1:A:606:ASN:OD1	1:A:606:ASN:N	2.49	0.41
1:A:546:ALA:O	1:A:547:GLY:C	2.63	0.41
1:A:80:TRP:HA	1:A:83:PHE:CE2	2.55	0.41
1:B:2:ASP:HA	1:B:3:PRO:HD3	1.96	0.41
1:A:95:VAL:C	1:A:97:THR:H	2.27	0.41
1:A:580:TRP:O	1:A:584:GLN:HG2	2.21	0.41
1:B:172:LYS:N	1:B:173:PRO:HD2	2.36	0.41
1:B:397:LEU:HD23	1:B:397:LEU:HA	1.85	0.41
1:B:14:GLU:OE1	1:B:85:ASP:HB3	2.21	0.41
1:B:98:LEU:HD12	1:B:98:LEU:N	2.35	0.41
1:B:172:LYS:HB3	1:B:173:PRO:HD3	2.02	0.41
1:B:248:ILE:O	1:B:473:ILE:HA	2.21	0.41
1:B:368:TYR:CE1	1:B:544:LEU:HA	2.56	0.41
1:A:92:ILE:HG22	1:A:93:GLY:N	2.35	0.40
1:A:321:LYS:HD2	1:A:330:CYS:SG	2.61	0.40
1:A:376:PRO:O	1:A:377:VAL:C	2.63	0.40
1:A:378:SER:O	1:A:381:ARG:HD2	2.22	0.40
1:A:390:ALA:O	1:A:394:VAL:HG23	2.21	0.40
1:A:270:PRO:O	1:A:272:PRO:HD2	2.21	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	600/628 (96%)	583 (97%)	15 (2%)	2 (0%)	36	29
1	B	596/628 (95%)	582 (98%)	12 (2%)	2 (0%)	36	29
All	All	1196/1256 (95%)	1165 (97%)	27 (2%)	4 (0%)	36	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	ILE
1	B	45	ASN
1	A	79	ILE
1	B	78	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	519/540 (96%)	503 (97%)	16 (3%)	35	29
1	B	517/540 (96%)	499 (96%)	18 (4%)	32	24
All	All	1036/1080 (96%)	1002 (97%)	34 (3%)	33	26

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	73	LYS

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Mol	Chain	Res	Type
1	A	82	GLN
1	A	90	ARG
1	A	92	ILE
1	A	96	ARG
1	A	152	SER
1	A	262	GLU
1	A	273	ASP
1	A	372	TYR
1	A	376	PRO
1	A	377	VAL
1	A	388	HIS
1	A	414	VAL
1	A	496	THR
1	A	517	LYS
1	B	23	SER
1	B	30	GLN
1	B	52	ARG
1	B	60	LEU
1	B	73	LYS
1	B	74	GLU
1	B	82	GLN
1	B	87	GLN
1	B	128	CYS
1	B	135	THR
1	B	152	SER
1	B	269	VAL
1	B	372	TYR
1	B	388	HIS
1	B	421	ASP
1	B	517	LYS
1	B	598	GLN
1	B	606	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	292	HIS
1	B	9	GLN
1	B	30	GLN
1	B	582	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

9 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	D	1	2,1	14,14,15	0.50	0	17,19,21	1.46	5 (29%)
2	FUC	D	2	2	10,10,11	0.52	0	14,14,16	1.41	1 (7%)
3	NAG	F	1	1,3	14,14,15	0.61	0	17,19,21	1.29	3 (17%)
3	NAG	F	2	3	14,14,15	0.36	0	17,19,21	1.23	3 (17%)
3	BMA	F	3	3	11,11,12	0.80	1 (9%)	15,15,17	1.99	3 (20%)
3	FUC	F	4	3	10,10,11	0.43	0	14,14,16	1.02	1 (7%)
4	NAG	G	1	1,4	14,14,15	0.67	0	17,19,21	1.51	4 (23%)
4	NAG	G	2	4	14,14,15	0.37	0	17,19,21	1.16	2 (11%)
4	BMA	G	3	4	11,11,12	0.84	0	15,15,17	1.34	4 (26%)

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
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	FUC	D	2	2	-	-	0/1/1/1
3	NAG	F	1	1,3	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	FUC	F	4	3	-	-	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	3	BMA	C2-C3	2.26	1.55	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	3	BMA	C1-C2-C3	6.03	118.43	109.64
2	D	2	FUC	O2-C2-C3	4.71	119.91	110.15
3	F	3	BMA	C2-C3-C4	3.38	116.81	110.86
4	G	1	NAG	C1-C2-N2	3.28	115.60	110.43
4	G	2	NAG	C1-O5-C5	3.24	116.52	112.19
4	G	1	NAG	C2-N2-C7	3.13	127.09	122.90
2	D	1	NAG	C1-O5-C5	2.74	115.86	112.19
4	G	3	BMA	C1-C2-C3	2.66	113.52	109.64
3	F	2	NAG	C2-N2-C7	-2.64	119.36	122.90
3	F	1	NAG	C1-C2-N2	2.62	114.56	110.43
3	F	1	NAG	C1-O5-C5	2.61	115.69	112.19
2	D	1	NAG	O6-C6-C5	2.58	120.13	111.33
3	F	2	NAG	C1-C2-N2	2.58	114.49	110.43
4	G	3	BMA	O2-C2-C3	2.29	114.89	110.15
3	F	3	BMA	C3-C4-C5	2.28	114.37	110.23
4	G	3	BMA	C1-O5-C5	2.27	115.23	112.19
3	F	4	FUC	O2-C2-C3	2.26	114.83	110.15
2	D	1	NAG	O5-C1-C2	-2.26	107.80	111.29
2	D	1	NAG	C1-C2-N2	2.26	113.99	110.43
3	F	2	NAG	O3-C3-C2	-2.25	104.73	109.40
2	D	1	NAG	O4-C4-C3	-2.23	105.13	110.38
4	G	1	NAG	C1-O5-C5	2.22	115.16	112.19
4	G	2	NAG	C1-C2-N2	2.21	113.92	110.43
4	G	3	BMA	O3-C3-C2	2.09	114.32	110.05
4	G	1	NAG	O3-C3-C2	2.05	113.65	109.40
3	F	1	NAG	O4-C4-C3	-2.05	105.56	110.38

There are no chirality outliers.

All (13) torsion outliers are listed below:

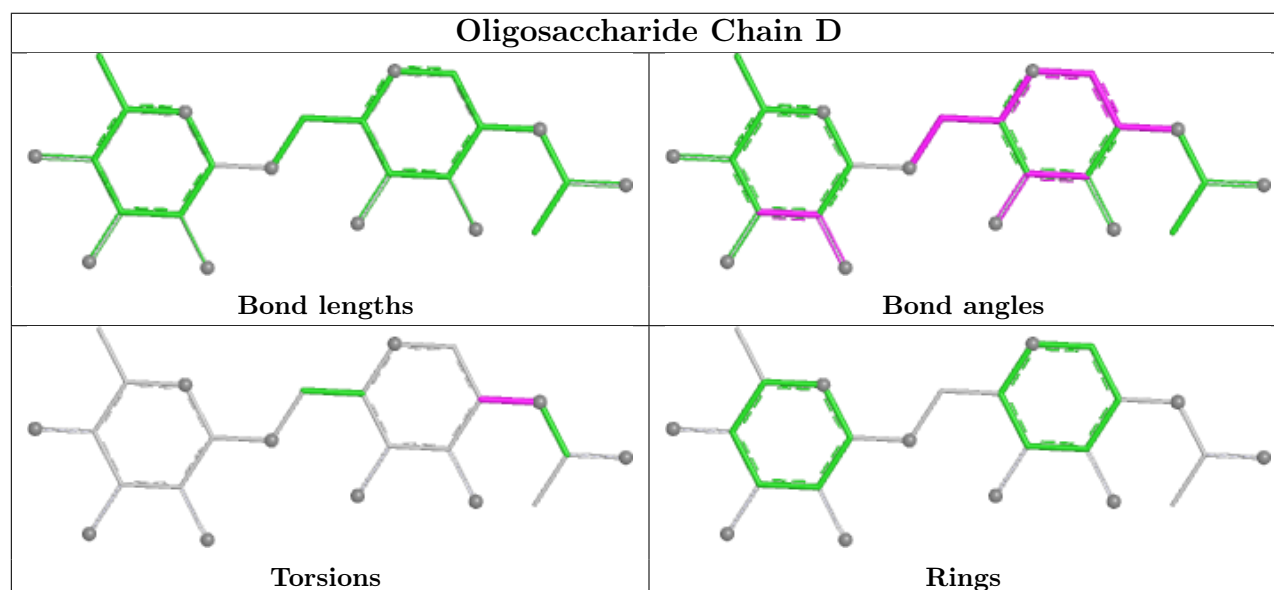
Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C1-C2-N2-C7
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
3	F	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
4	G	3	BMA	O5-C5-C6-O6
4	G	3	BMA	C4-C5-C6-O6
3	F	1	NAG	C8-C7-N2-C2
2	D	1	NAG	C3-C2-N2-C7

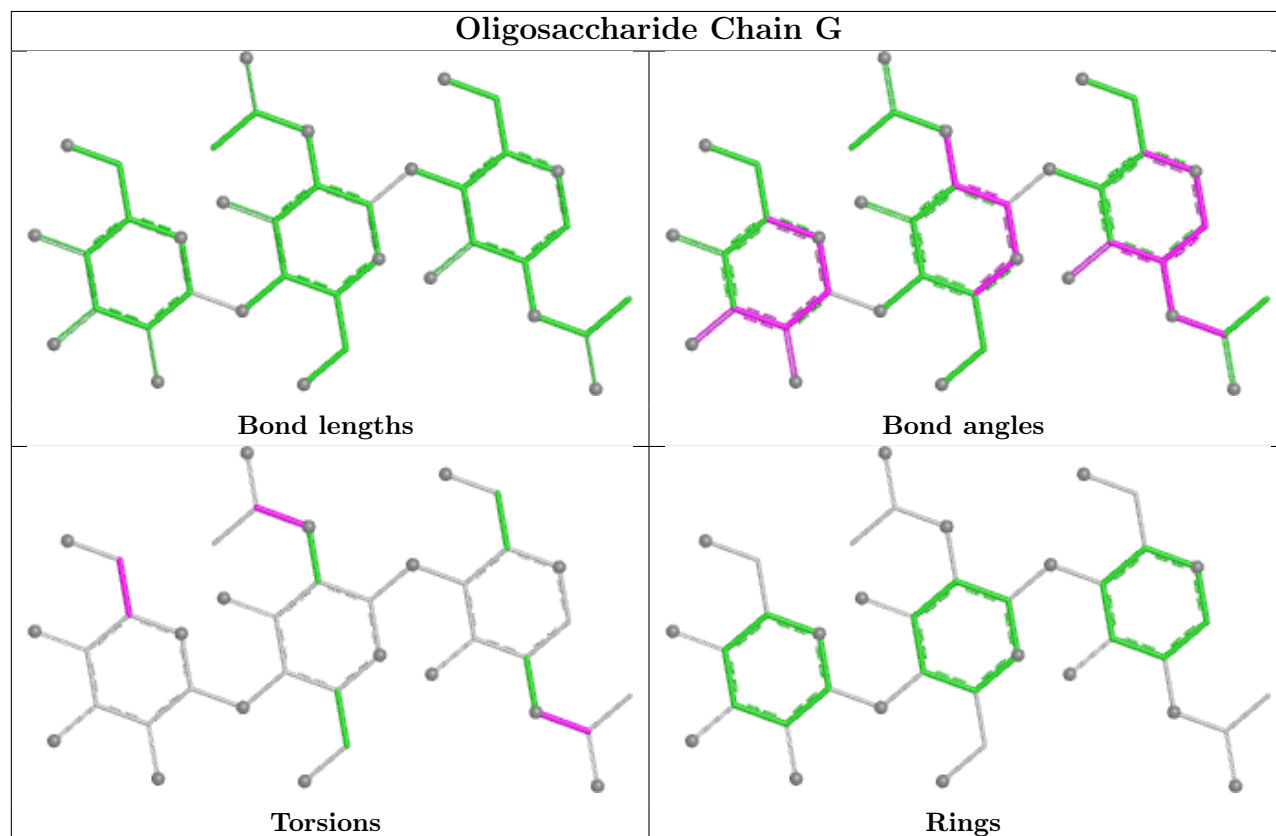
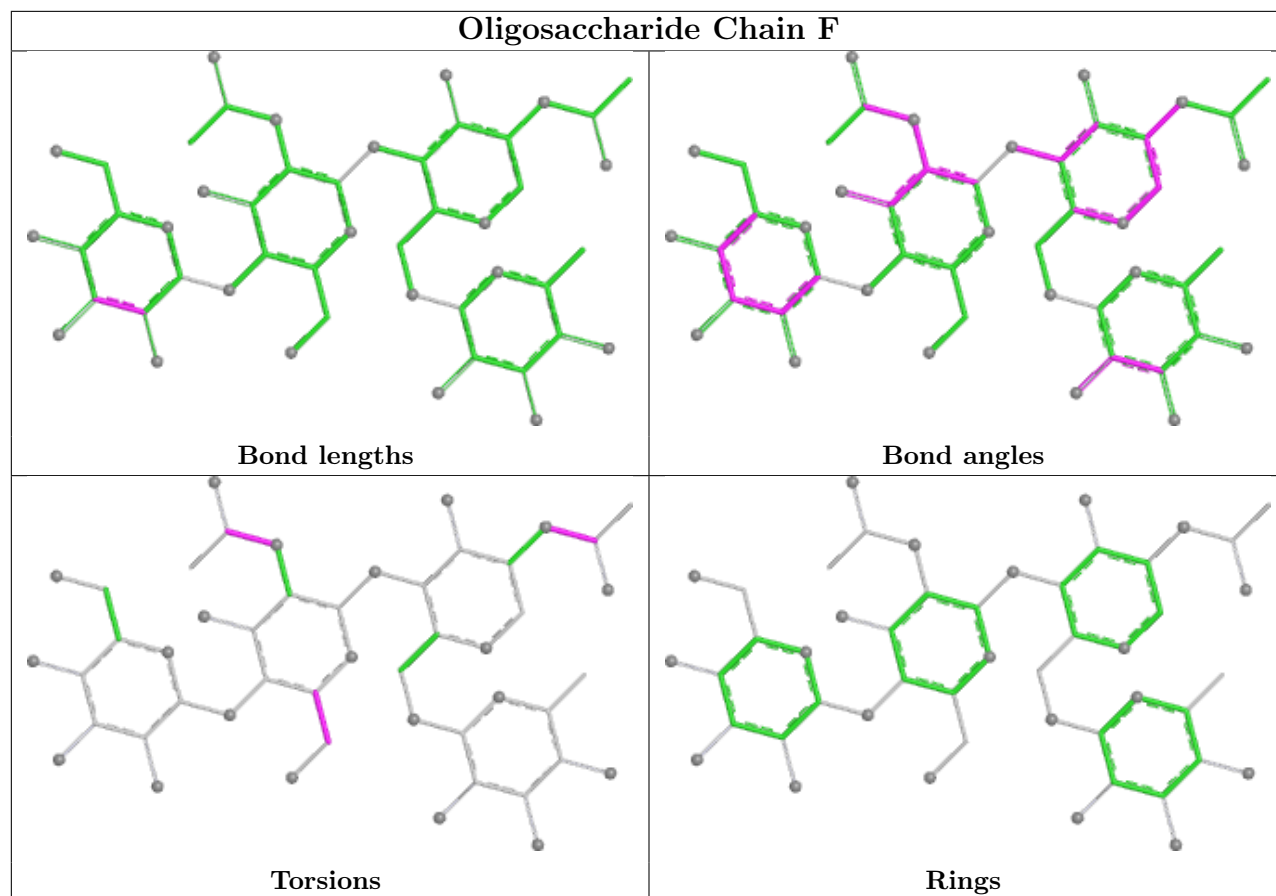
There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	3	BMA	1	0
4	G	2	NAG	1	0
4	G	1	NAG	1	0

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





5.6 Ligand geometry

Of 16 ligands modelled in this entry, 5 are monoatomic - leaving 11 for Mogul analysis.

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	708	1	14,14,15	0.62	0	17,19,21	1.78	5 (29%)
5	NAG	A	701	1	14,14,15	0.54	0	17,19,21	1.22	2 (11%)
11	PG4	B	702	-	12,12,12	0.38	0	11,11,11	0.28	0
7	PEG	B	703	-	6,6,6	0.28	0	5,5,5	0.16	0
7	PEG	A	703	-	6,6,6	0.20	0	5,5,5	0.32	0
7	PEG	A	704	-	6,6,6	0.37	0	5,5,5	0.24	0
10	A1IJZ	A	709	8	35,35,35	3.02	14 (40%)	42,49,49	1.90	10 (23%)
10	A1IJZ	B	707	8	35,35,35	3.05	12 (34%)	42,49,49	1.96	11 (26%)
6	P33	A	702	-	21,21,21	0.25	0	20,20,20	0.27	0
5	NAG	B	701	1	14,14,15	0.34	0	17,19,21	0.83	0
7	PEG	A	705	-	6,6,6	0.35	0	5,5,5	0.26	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	708	1	-	4/6/23/26	0/1/1/1
5	NAG	A	701	1	-	0/6/23/26	0/1/1/1
11	PG4	B	702	-	-	6/10/10/10	-
7	PEG	B	703	-	-	4/4/4/4	-
7	PEG	A	703	-	-	2/4/4/4	-
7	PEG	A	704	-	-	1/4/4/4	-
10	A1IJZ	A	709	8	-	4/36/56/56	0/3/3/3
10	A1IJZ	B	707	8	-	6/36/56/56	0/3/3/3
6	P33	A	702	-	-	12/19/19/19	-
5	NAG	B	701	1	-	2/6/23/26	0/1/1/1
7	PEG	A	705	-	-	0/4/4/4	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	709	A1IJZ	C07-C06	-9.66	1.37	1.53
10	B	707	A1IJZ	C07-C06	-8.55	1.39	1.53
10	B	707	A1IJZ	C06-N10	8.20	1.56	1.46
10	A	709	A1IJZ	C06-N10	6.30	1.54	1.46
10	B	707	A1IJZ	C30-N26	5.45	1.57	1.47
10	B	707	A1IJZ	C11-N10	5.44	1.46	1.34
10	B	707	A1IJZ	C09-N10	-5.36	1.37	1.47
10	A	709	A1IJZ	C09-N10	-5.10	1.37	1.47
10	B	707	A1IJZ	C29-C30	-5.07	1.41	1.53
10	A	709	A1IJZ	C29-C30	-4.77	1.42	1.53
10	B	707	A1IJZ	C02-N26	4.41	1.44	1.34
10	A	709	A1IJZ	C11-N10	4.39	1.44	1.34
10	A	709	A1IJZ	C02-N26	4.33	1.44	1.34
10	A	709	A1IJZ	C30-N26	4.20	1.55	1.47
10	A	709	A1IJZ	C27-N26	-4.02	1.39	1.47
10	A	709	A1IJZ	C05-C06	3.60	1.58	1.54
10	B	707	A1IJZ	C27-N26	-2.95	1.41	1.47
10	B	707	A1IJZ	C28-C29	2.54	1.62	1.51
10	A	709	A1IJZ	O32-C31	2.50	1.29	1.22
10	A	709	A1IJZ	C19-C20	2.49	1.43	1.38
10	A	709	A1IJZ	C17-C16	2.45	1.43	1.38
10	A	709	A1IJZ	C08-C07	2.26	1.61	1.51
10	B	707	A1IJZ	C08-C09	2.22	1.59	1.51
10	B	707	A1IJZ	O01-C02	-2.21	1.18	1.22
10	A	709	A1IJZ	C19-C18	2.13	1.42	1.38
10	B	707	A1IJZ	C17-C16	2.07	1.42	1.38

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	707	A1IJZ	C31-C30-N26	-5.77	100.97	112.54
10	A	709	A1IJZ	C31-C30-N26	-5.29	101.93	112.54
10	B	707	A1IJZ	O24-C22-O23	-5.23	112.21	124.08
5	A	708	NAG	C1-O5-C5	4.67	118.44	112.19
10	B	707	A1IJZ	O33-C31-O32	-4.21	114.52	124.08
10	B	707	A1IJZ	O24-C22-C05	4.21	128.76	114.15
10	A	709	A1IJZ	O33-C31-O32	-4.15	114.66	124.08
10	A	709	A1IJZ	O33-C31-C30	4.03	126.49	113.34
10	A	709	A1IJZ	C29-C30-N26	3.67	108.39	103.02
10	A	709	A1IJZ	C07-C06-N10	-3.36	99.84	102.66
5	A	708	NAG	C1-C2-N2	3.24	115.54	110.43
5	A	701	NAG	C1-O5-C5	3.21	116.48	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	709	A1IJZ	C27-N26-C30	-2.94	107.39	112.01
10	A	709	A1IJZ	O24-C22-C05	2.68	123.43	114.15
10	A	709	A1IJZ	C25-C03-N04	-2.62	103.37	108.89
10	B	707	A1IJZ	C28-C27-N26	2.47	107.49	103.24
10	B	707	A1IJZ	O33-C31-C30	2.44	121.31	113.34
10	A	709	A1IJZ	C28-C27-N26	2.42	107.40	103.24
5	A	708	NAG	C2-N2-C7	-2.41	119.67	122.90
10	B	707	A1IJZ	C29-C30-C31	2.30	116.16	111.26
10	B	707	A1IJZ	C20-C15-C16	2.25	121.57	118.23
10	A	709	A1IJZ	C15-C14-C12	-2.18	109.67	114.13
5	A	708	NAG	O6-C6-C5	2.14	118.61	111.33
10	B	707	A1IJZ	C14-C12-C11	-2.08	103.86	109.43
5	A	701	NAG	O3-C3-C2	-2.06	105.13	109.40
5	A	708	NAG	O3-C3-C4	2.02	115.15	110.38
10	B	707	A1IJZ	C29-C30-N26	2.01	105.97	103.02
10	B	707	A1IJZ	C28-C29-C30	2.00	108.31	104.14

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	707	A1IJZ	C22-C05-N04-C03
10	B	707	A1IJZ	C22-C05-C06-C07
11	B	702	PG4	O3-C5-C6-O4
6	A	702	P33	O16-C17-C18-O19
6	A	702	P33	O13-C14-C15-O16
7	B	703	PEG	O2-C3-C4-O4
7	A	704	PEG	O2-C3-C4-O4
7	A	703	PEG	O1-C1-C2-O2
6	A	702	P33	O10-C11-C12-O13
5	A	708	NAG	C4-C5-C6-O6
11	B	702	PG4	O1-C1-C2-O2
7	A	703	PEG	C4-C3-O2-C2
10	A	709	A1IJZ	C22-C05-C06-C07
6	A	702	P33	O1-C2-C3-O4
7	B	703	PEG	O1-C1-C2-O2
6	A	702	P33	C17-C18-O19-C20
7	B	703	PEG	C1-C2-O2-C3
5	B	701	NAG	C4-C5-C6-O6
10	A	709	A1IJZ	N04-C05-C06-C07
5	A	708	NAG	C3-C2-N2-C7
10	B	707	A1IJZ	C22-C05-C06-N10

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Mol	Chain	Res	Type	Atoms
7	B	703	PEG	C4-C3-O2-C2
6	A	702	P33	O19-C20-C21-O22
10	A	709	A1IJZ	N04-C05-C22-O24
10	B	707	A1IJZ	N04-C05-C22-O24
6	A	702	P33	C12-C11-O10-C9
11	B	702	PG4	C4-C3-O2-C2
6	A	702	P33	C14-C15-O16-C17
11	B	702	PG4	C8-C7-O4-C6
11	B	702	PG4	C3-C4-O3-C5
10	A	709	A1IJZ	N04-C05-C22-O23
10	B	707	A1IJZ	N04-C05-C22-O23
6	A	702	P33	C18-C17-O16-C15
5	A	708	NAG	C1-C2-N2-C7
6	A	702	P33	C21-C20-O19-C18
6	A	702	P33	C8-C9-O10-C11
5	A	708	NAG	O5-C5-C6-O6
6	A	702	P33	O7-C8-C9-O10
11	B	702	PG4	O2-C3-C4-O3
5	B	701	NAG	C8-C7-N2-C2
10	B	707	A1IJZ	N04-C05-C06-C07

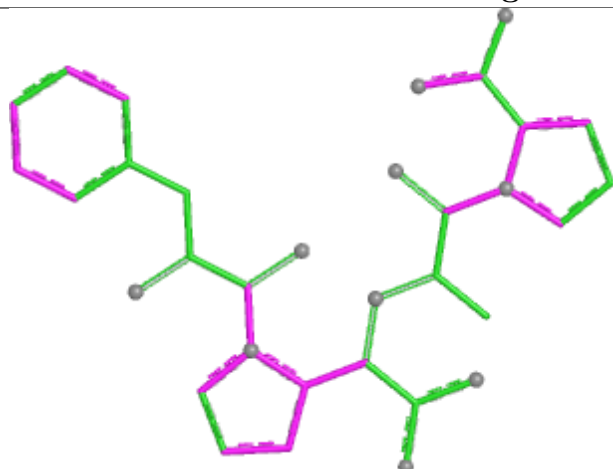
There are no ring outliers.

3 monomers are involved in 9 short contacts:

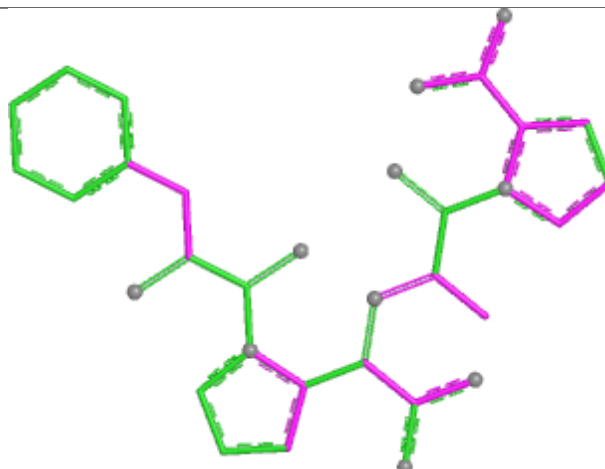
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	702	PG4	5	0
7	A	704	PEG	1	0
6	A	702	P33	3	0

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.

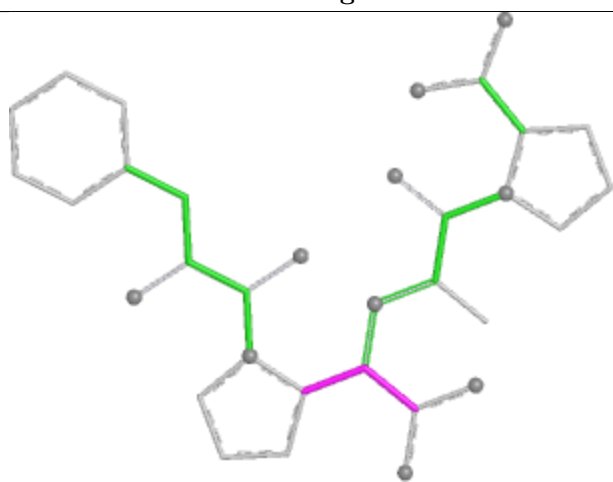
Ligand A1IJZ A 709



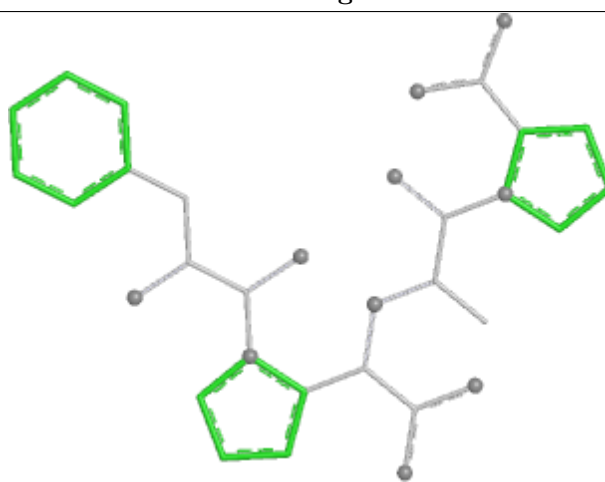
Bond lengths



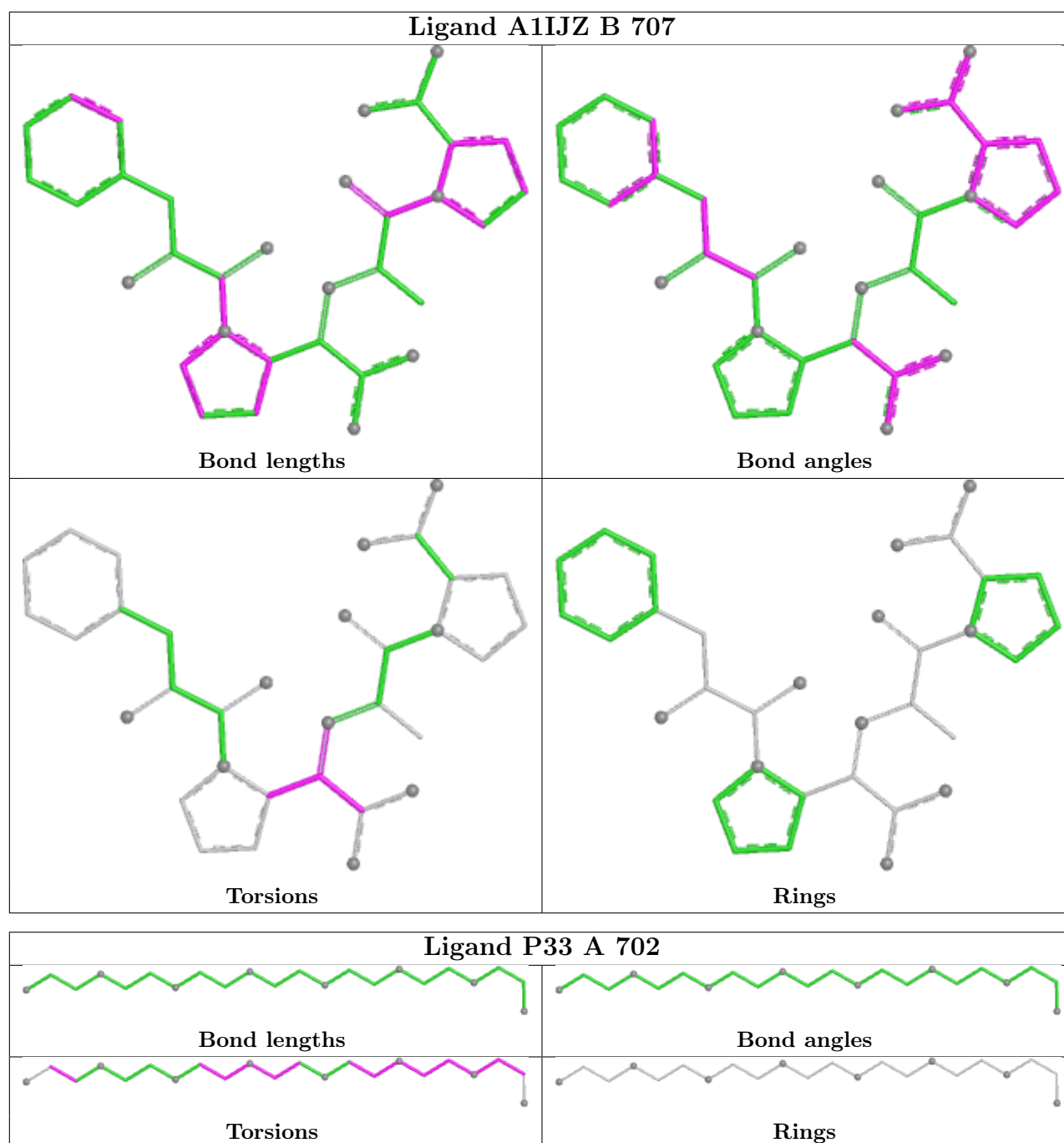
Bond angles



Torsions



Rings



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	604/628 (96%)	-0.19	25 (4%) 41 44	18, 31, 56, 86	0
1	B	602/628 (95%)	0.08	36 (5%) 27 29	19, 37, 75, 110	0
All	All	1206/1256 (96%)	-0.06	61 (5%) 33 36	18, 34, 67, 110	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	134	ALA	5.7
1	B	15	ALA	5.1
1	B	129	LEU	4.2
1	B	79	ILE	4.1
1	A	607	TYR	3.9
1	B	8	GLY	3.9
1	B	83	PHE	3.8
1	B	86	PRO	3.8
1	A	129	LEU	3.4
1	B	414	VAL	3.3
1	B	80	TRP	3.3
1	A	72	ALA	3.3
1	B	93	GLY	3.3
1	A	91	ILE	3.2
1	B	17	ALA	3.2
1	A	92	ILE	3.1
1	B	13	ASP	2.9
1	A	94	ALA	2.8
1	A	24	TYR	2.8
1	A	86	PRO	2.8
1	B	78	PRO	2.7
1	A	80	TRP	2.7
1	A	88	LEU	2.7
1	A	78	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	135	THR	2.6
1	B	20	PHE	2.6
1	B	19	LEU	2.6
1	B	92	ILE	2.6
1	B	10	PHE	2.5
1	B	11	SER	2.5
1	A	95	VAL	2.5
1	B	16	GLY	2.5
1	B	64	PHE	2.4
1	A	15	ALA	2.4
1	A	414	VAL	2.4
1	B	606	ASN	2.4
1	B	12	ALA	2.3
1	A	25	GLN	2.3
1	B	9	GLN	2.3
1	B	5	LEU	2.3
1	B	135	THR	2.3
1	A	12	ALA	2.3
1	A	325	GLY	2.3
1	B	91	ILE	2.3
1	B	84	THR	2.3
1	B	379	LEU	2.3
1	A	93	GLY	2.2
1	B	72	ALA	2.2
1	B	89	ARG	2.2
1	A	19	LEU	2.2
1	B	2	ASP	2.2
1	A	83	PHE	2.2
1	B	52	ARG	2.2
1	A	79	ILE	2.1
1	A	84	THR	2.1
1	A	14	GLU	2.1
1	B	59	LEU	2.1
1	B	75	LEU	2.1
1	B	136	CYS	2.1
1	B	325	GLY	2.0
1	B	88	LEU	2.0

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

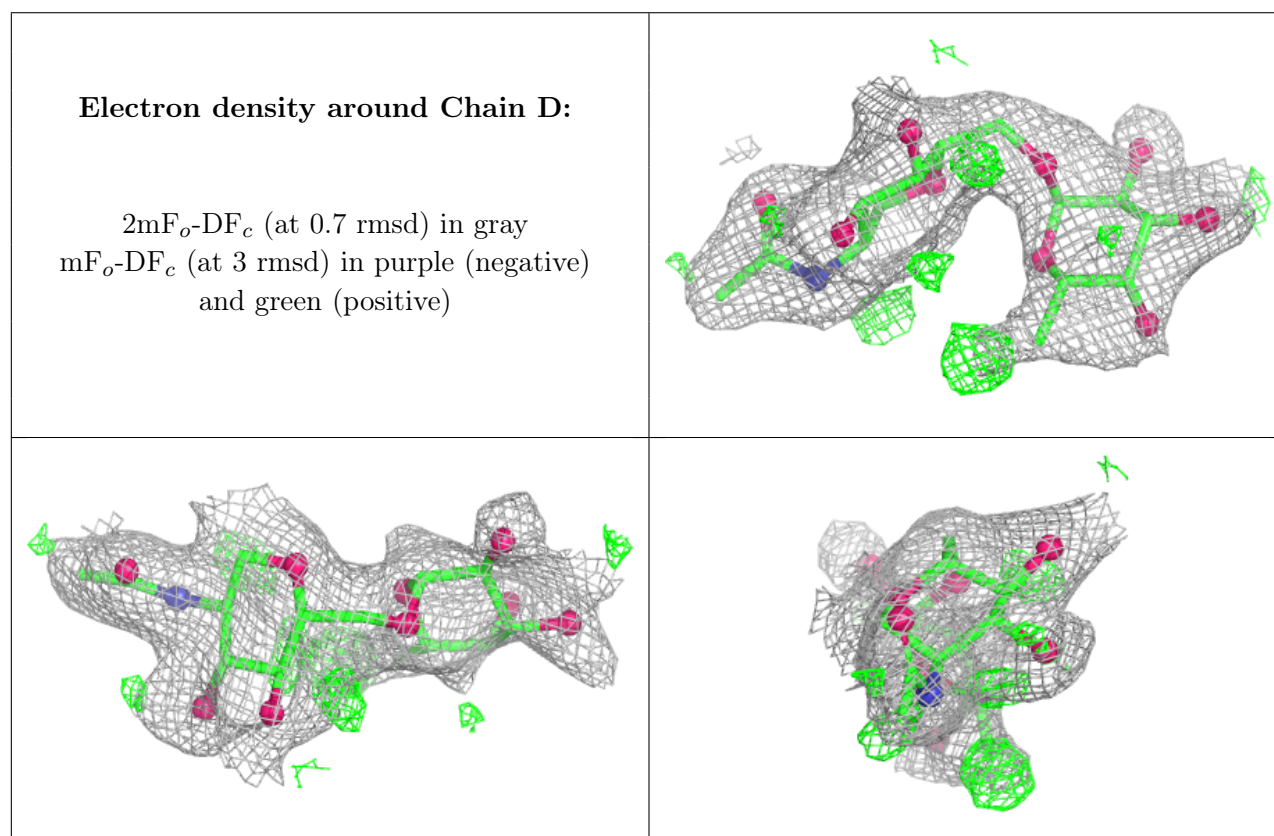
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [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.

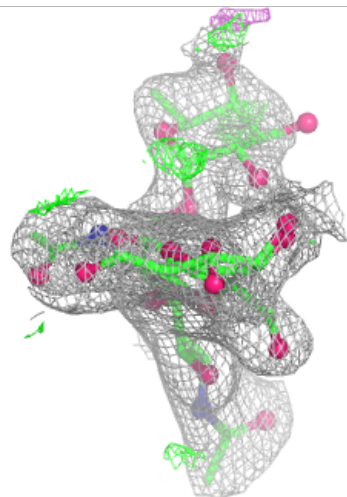
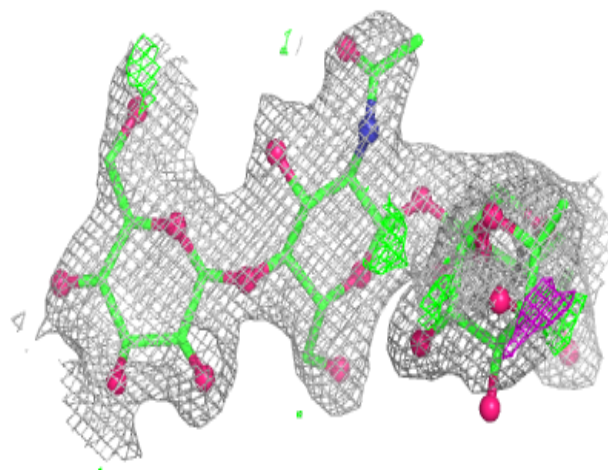
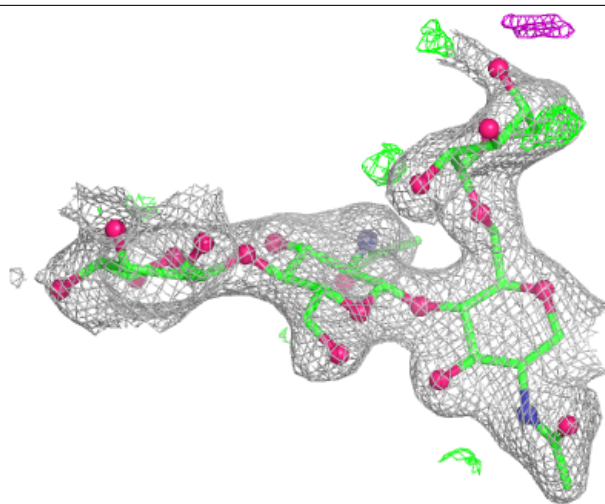
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	D	1	14/15	0.95	0.07	33,46,57,58	0
2	FUC	D	2	10/11	-	-	69,78,85,88	0
3	NAG	F	1	14/15	-	-	34,41,56,60	0
3	NAG	F	2	14/15	-	-	40,51,63,70	0
3	BMA	F	3	11/12	-	-	60,65,73,74	0
3	FUC	F	4	10/11	-	-	43,48,51,59	10
4	NAG	G	1	14/15	-	-	52,60,77,77	0
4	NAG	G	2	14/15	-	-	55,69,79,80	0
4	BMA	G	3	11/12	-	-	77,89,97,105	0

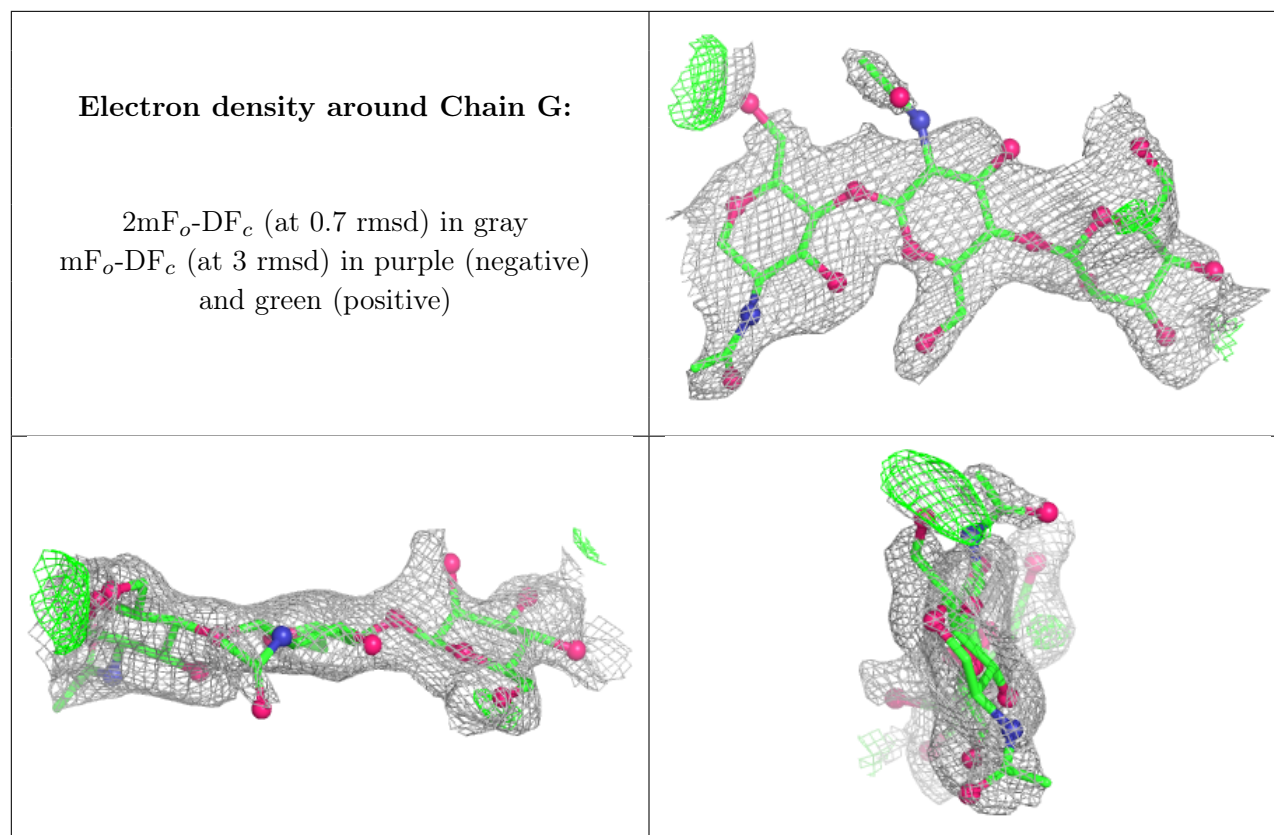
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain F:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	B	701	14/15	0.85	0.11	64,66,74,77	0
7	PEG	A	703	7/7	0.87	0.12	55,60,64,65	0
7	PEG	A	705	7/7	0.87	0.14	43,47,55,65	0
7	PEG	B	703	7/7	0.90	0.12	46,57,62,63	0
5	NAG	A	708	14/15	0.91	0.10	35,40,53,59	0
5	NAG	A	701	14/15	0.92	0.08	45,51,52,54	0
11	PG4	B	702	13/13	0.92	0.10	45,49,59,60	0
6	P33	A	702	22/22	0.93	0.12	51,59,74,79	0
7	PEG	A	704	7/7	0.94	0.10	48,51,57,61	0
10	A1IJZ	A	709	33/33	0.95	0.08	24,28,46,49	0
10	A1IJZ	B	707	33/33	0.96	0.07	22,27,43,50	0
9	CL	B	705	1/1	0.99	0.02	26,26,26,26	0
8	ZN	A	706	1/1	0.99	0.02	21,21,21,21	0
8	ZN	B	704	1/1	0.99	0.03	21,21,21,21	0

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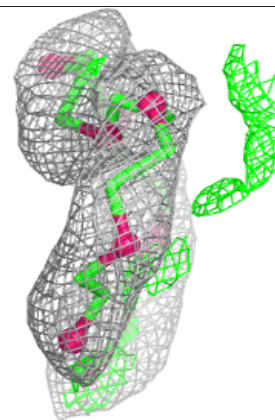
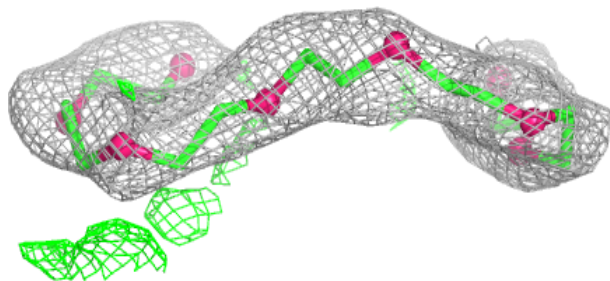
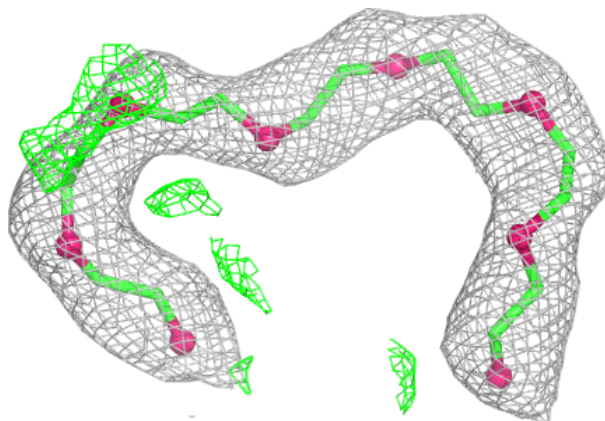
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	CL	A	707	1/1	0.99	0.06	23,23,23,23	0
12	MG	B	706	1/1	0.99	0.06	38,38,38,38	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.

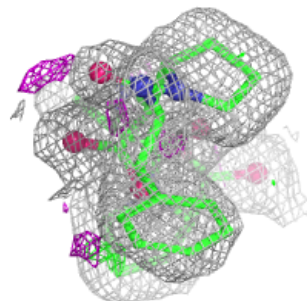
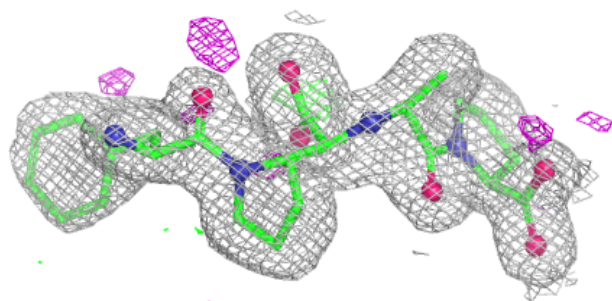
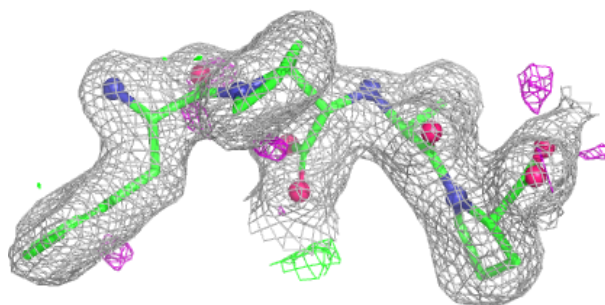
Electron density around P33 A 702:

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

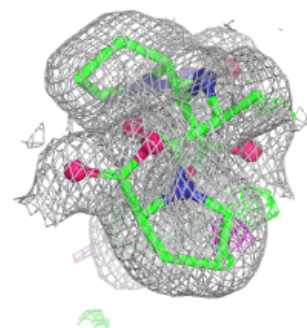
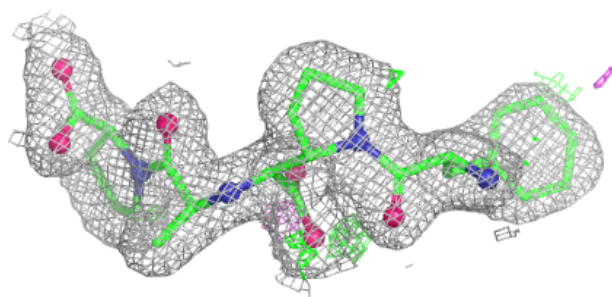
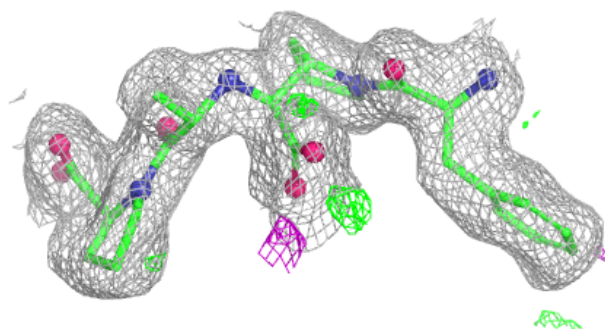


Electron density around A1IJZ A 709:

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

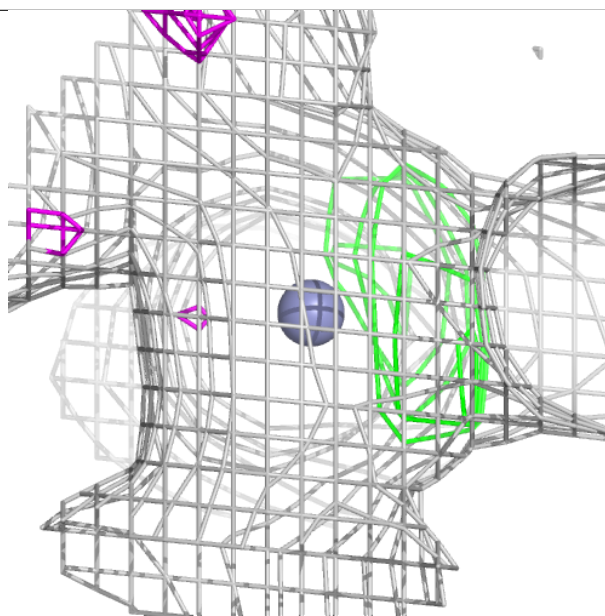
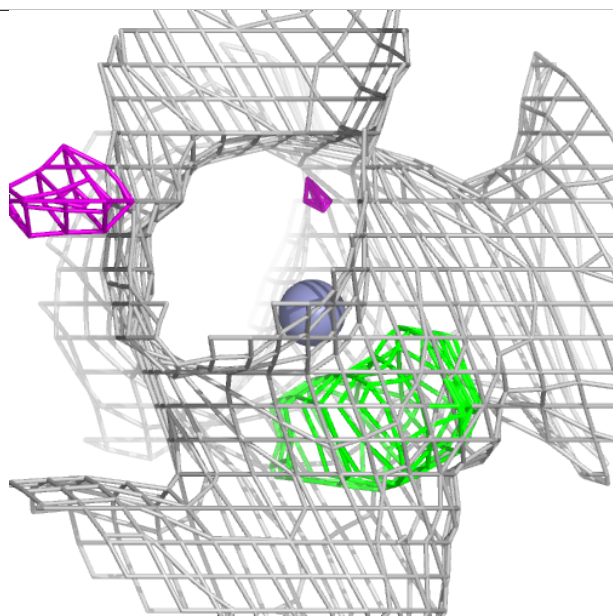
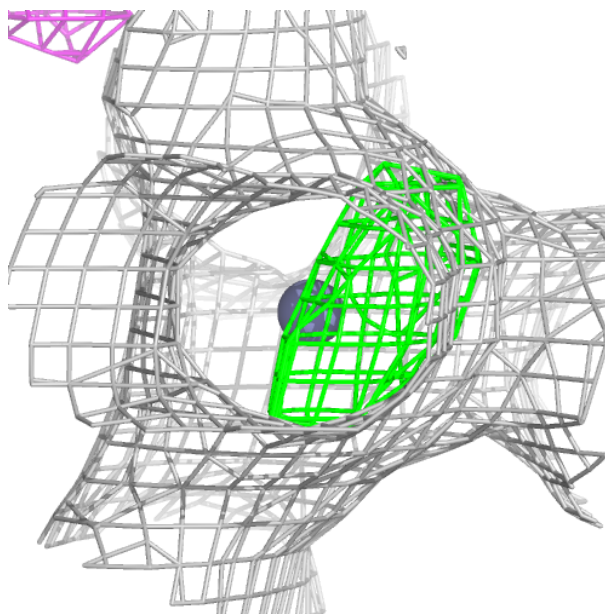
**Electron density around A1IJZ B 707:**

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



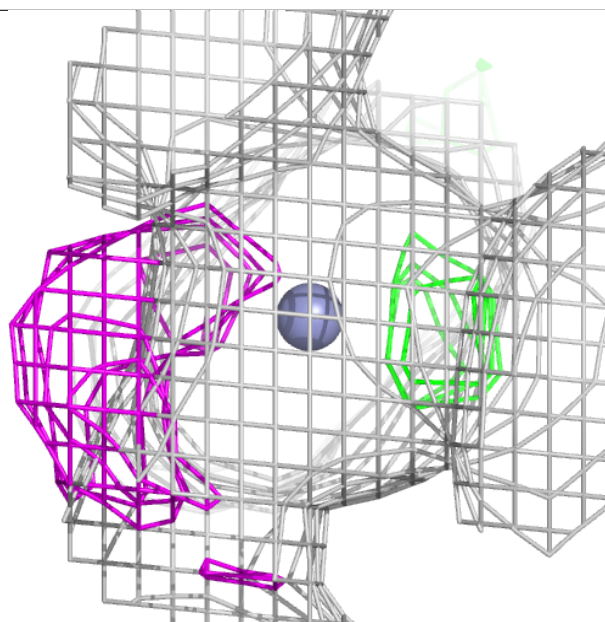
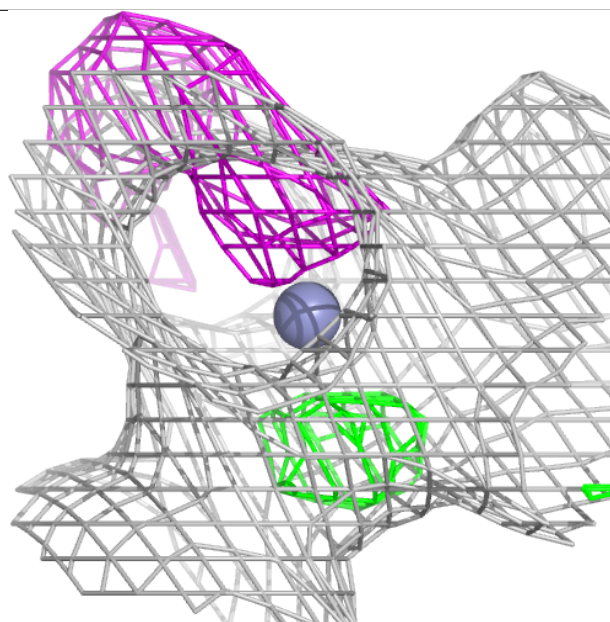
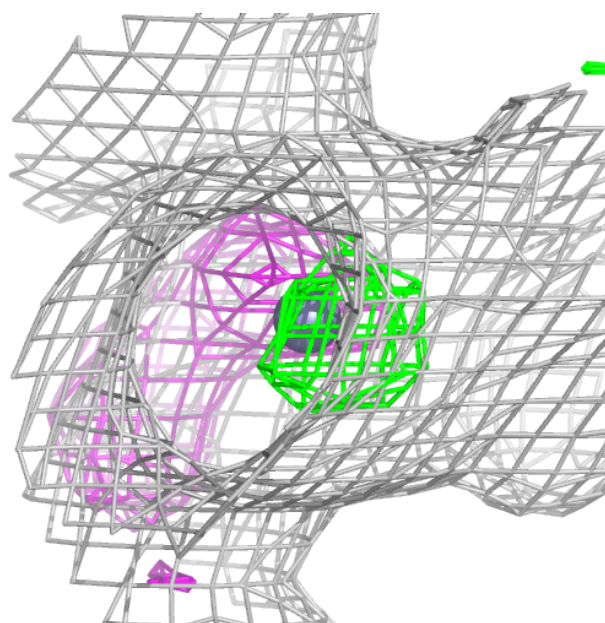
Electron density around ZN A 706:

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



Electron density around ZN B 704:

$2mF_o-DF_c$ (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.