



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:02 AM UTC

PDB ID : 9GBS / pdb_00009gbs
Title : Human Angiotensin-1 converting enzyme N-domain in complex with a diprolyl inhibitor- SG18
Authors : Gregory, K.S.; Cozier, G.E.; Acharya, K.R.
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

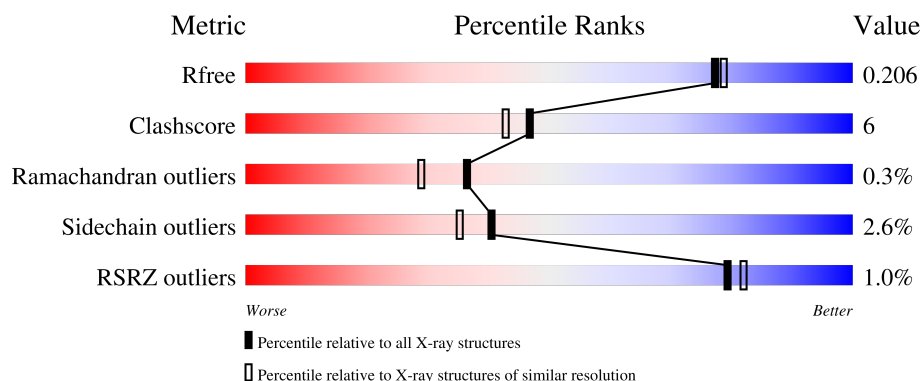
1 Overall quality at a glance

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	79% 15% ...
1	B	628	81% 14% ...
2	F	2	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
8	NAG	B	811	-	-	X	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 11058 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	603	Total	C	N	O	S	0	13	0
			5023	3219	865	919	20			
1	B	603	Total	C	N	O	S	0	6	0
			4987	3200	860	908	19			

There are 16 discrepancies between the modelled and reference sequences:

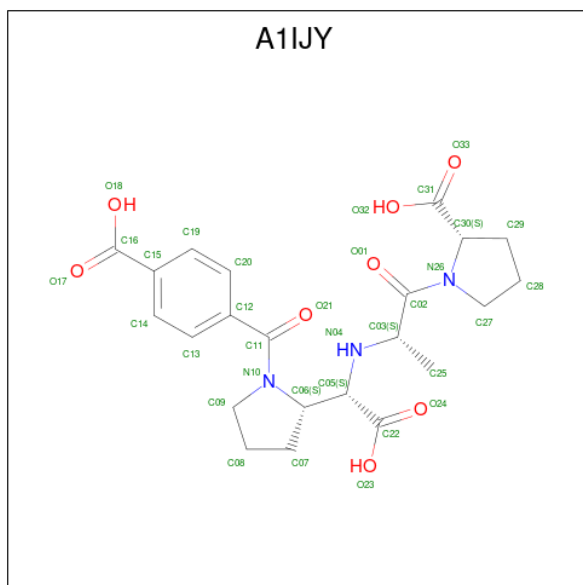
Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	engineered mutation	UNP P12821
A	25	GLN	ASN	engineered mutation	UNP P12821
A	82	GLN	ASN	engineered mutation	UNP P12821
A	117	GLN	ASN	engineered mutation	UNP P12821
A	131	GLN	ASN	engineered mutation	UNP P12821
A	289	GLN	ASN	engineered mutation	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.



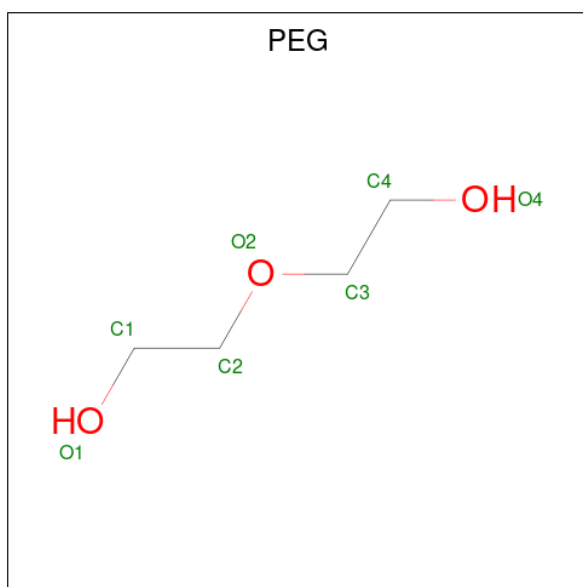
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 3 is (2S)-1-[(2S)-2-[[[(1S)-1-[(2S)-1-(4-carboxyphenyl)carbonylpyrrolidin-2-yl]-2-oxidanyl-2-oxidanylidene-ethyl]amino]propanoyl]pyrrolidine-2-carboxylic acid (CCD ID: A1IJY) (formula: C₂₂H₂₇N₃O₈).



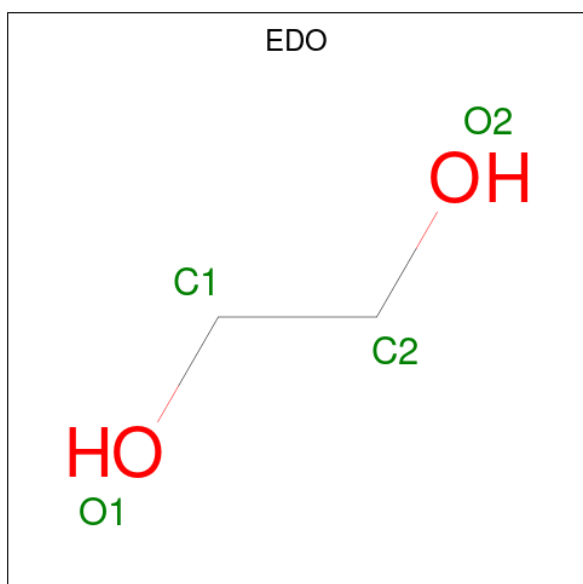
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			33	22	3	8		
3	B	1	Total	C	N	O	0	0
			33	22	3	8		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



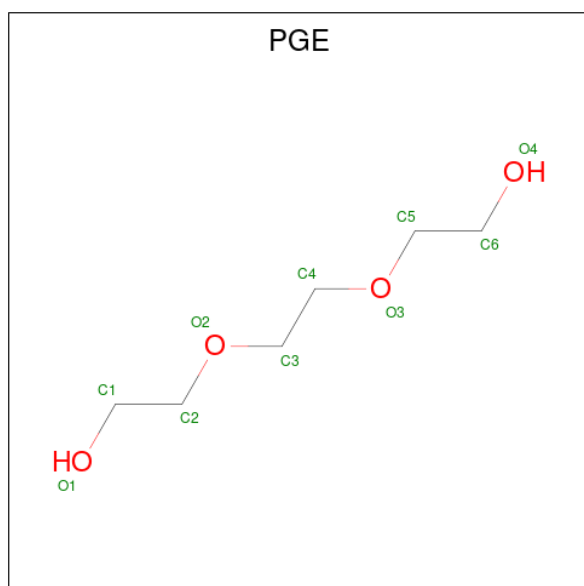
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



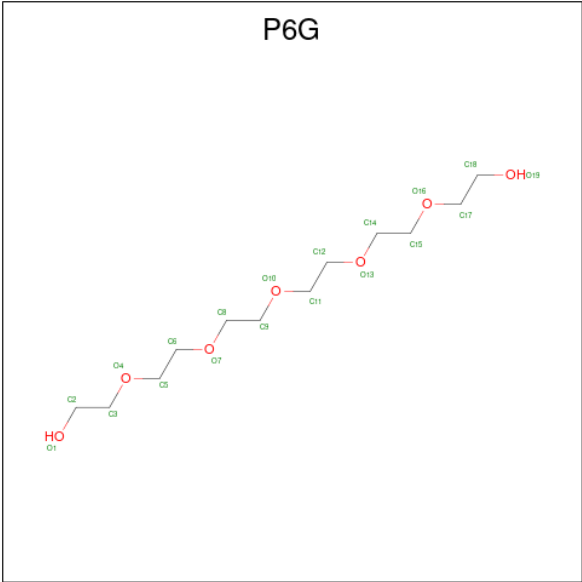
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



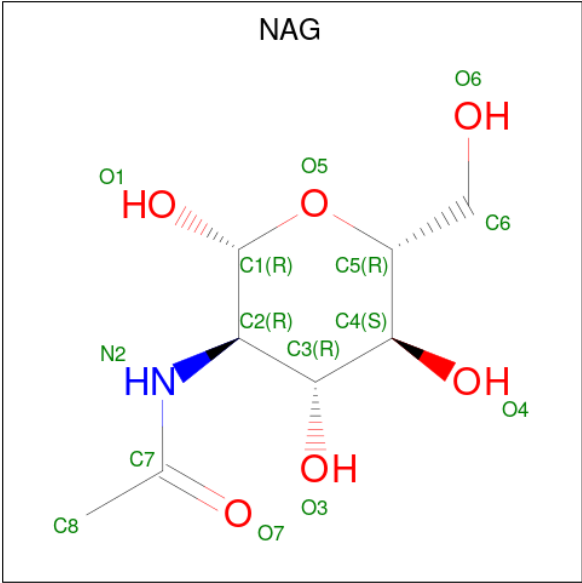
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		
6	A	1	Total	C	O	0	0
			10	6	4		
6	A	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			19	12	7		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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

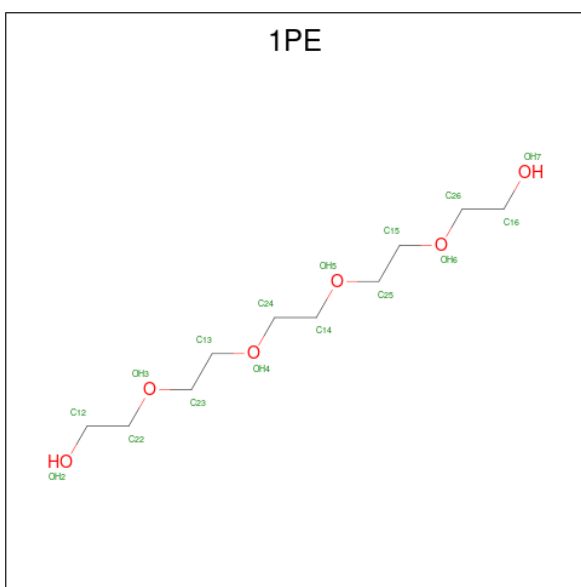
- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

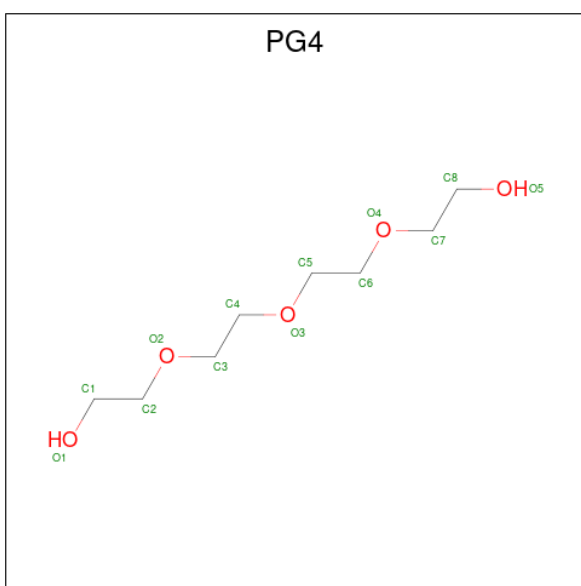
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	Cl	0	0
			1	1		
10	B	1	Total	Cl	0	0
			1	1		

- Molecule 11 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



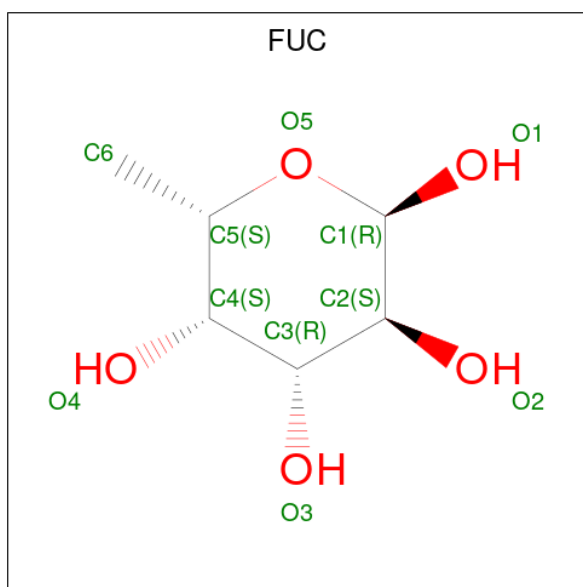
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			16	10	6		
11	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 12 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



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

- Molecule 13 is alpha-L-fucopyranose (CCD ID: FUC) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	B	1	Total	C	O	0	0
			10	6	4		

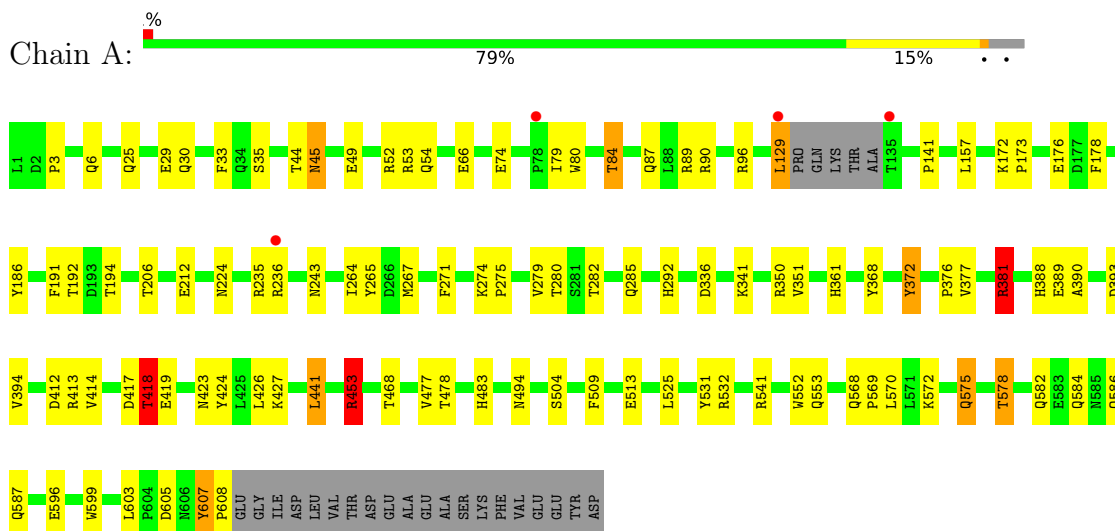
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	306	Total	O	0	0
			306	306		
14	B	353	Total	O	0	0
			353	353		

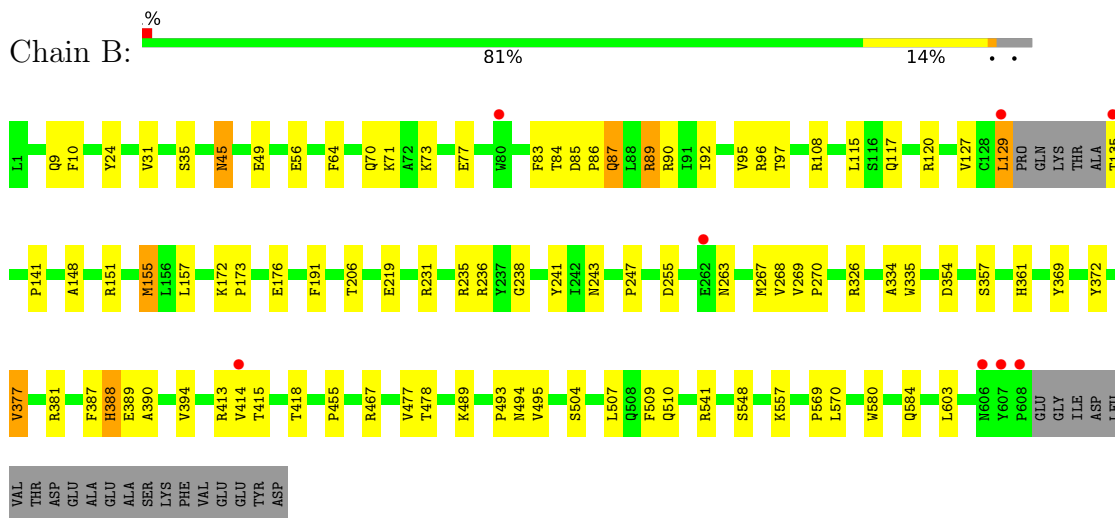
3 Residue-property plots

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



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



MAG1
FUC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.72Å 77.16Å 81.84Å 88.37° 64.58° 75.25°	Depositor
Resolution (Å)	63.72 – 1.90 63.72 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.8 (63.72-1.90) 97.7 (63.72-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.165 , 0.204 0.166 , 0.206	Depositor DCC
R_{free} test set	5879 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11058	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% 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: PEG, NAG, CL, EDO, 1PE, PG4, A1IJY, PGE, FUC, P6G, ZN

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	0.85	1/5181 (0.0%)	1.45	49/7054 (0.7%)
1	B	0.93	2/5142 (0.0%)	1.48	41/7001 (0.6%)
All	All	0.89	3/10323 (0.0%)	1.47	90/14055 (0.6%)

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	4
1	B	0	4
All	All	0	8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	455	PRO	CA-CB	6.02	1.62	1.54
1	A	361	HIS	ND1-CE1	5.34	1.37	1.32
1	B	388	HIS	CE1-NE2	5.33	1.37	1.32

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	85	ASP	CB-CA-C	11.25	123.01	110.08
1	A	418	THR	CA-CB-OG1	-9.57	95.24	109.60
1	A	87	GLN	CB-CA-C	-9.23	95.16	110.85
1	B	49	GLU	CB-CG-CD	8.94	127.79	112.60
1	B	206	THR	CA-CB-OG1	-8.68	96.58	109.60
1	A	607	TYR	CB-CA-C	8.49	121.72	109.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	PHE	CA-CB-CG	-7.97	105.83	113.80
1	B	418	THR	CA-CB-OG1	-7.71	98.03	109.60
1	B	387	PHE	CB-CA-C	-7.47	98.39	110.79
1	B	127	VAL	N-CA-CB	-7.32	101.29	111.25
1	B	263	ASN	CA-CB-CG	-7.25	105.35	112.60
1	A	192	THR	CA-CB-OG1	-6.97	99.15	109.60
1	A	377	VAL	N-CA-CB	6.96	119.17	110.47
1	B	361	HIS	CA-CB-CG	-6.75	107.05	113.80
1	A	336	ASP	CA-CB-CG	6.75	119.34	112.60
1	B	507	LEU	N-CA-CB	-6.72	99.86	110.28
1	A	212	GLU	CB-CG-CD	6.47	123.60	112.60
1	A	84	THR	CA-CB-OG1	-6.45	99.92	109.60
1	B	377	VAL	N-CA-CB	6.42	118.50	110.47
1	B	129	LEU	N-CA-CB	6.29	121.19	110.50
1	A	587	GLN	CB-CA-C	-6.28	100.01	110.68
1	A	282	THR	CA-CB-OG1	-6.25	100.22	109.60
1	B	108	ARG	N-CA-CB	6.23	119.05	110.01
1	B	494	ASN	CA-CB-CG	-6.15	106.45	112.60
1	A	178	PHE	CA-CB-CG	-6.10	107.70	113.80
1	B	176	GLU	CB-CA-C	-6.10	100.67	110.79
1	A	575	GLN	CB-CA-C	-6.08	98.31	110.42
1	A	381	ARG	CB-CG-CD	6.07	125.26	111.30
1	A	52	ARG	CD-NE-CZ	6.01	132.82	124.40
1	A	341	LYS	CB-CA-C	-5.96	100.59	110.37
1	B	270	PRO	N-CA-C	5.93	121.34	113.57
1	B	241	TYR	N-CA-CB	-5.86	102.04	110.65
1	A	66	GLU	CB-CG-CD	5.77	122.41	112.60
1	A	468	THR	CA-CB-OG1	-5.75	100.97	109.60
1	B	478	THR	CA-CB-OG1	-5.75	100.98	109.60
1	B	219	GLU	CB-CG-CD	5.70	122.29	112.60
1	A	509	PHE	CA-CB-CG	-5.62	108.18	113.80
1	A	224	ASN	CA-CB-CG	-5.61	106.99	112.60
1	A	586	GLN	N-CA-CB	5.59	118.28	109.94
1	B	415	THR	CA-CB-OG1	-5.58	101.24	109.60
1	A	351	VAL	N-CA-CB	-5.55	105.91	111.90
1	A	194	THR	CA-CB-OG1	-5.54	101.30	109.60
1	A	584	GLN	N-CA-CB	5.53	118.18	109.94
1	A	191	PHE	CA-CB-CG	-5.50	108.30	113.80
1	A	388	HIS	CB-CG-CD2	-5.49	124.06	131.20
1	A	553	GLN	N-CA-CB	5.49	118.79	110.28
1	A	29	GLU	N-CA-CB	5.48	118.28	110.06
1	B	87	GLN	CB-CA-C	5.46	119.86	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	85	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	478	THR	CA-CB-OG1	-5.42	101.46	109.60
1	A	186	TYR	N-CA-CB	5.41	118.66	110.28
1	A	393	ASP	CA-CB-CG	5.41	118.01	112.60
1	B	176	GLU	N-CA-CB	5.40	118.05	110.12
1	B	238	GLY	CA-C-N	5.38	129.21	120.60
1	B	238	GLY	C-N-CA	5.38	129.21	120.60
1	B	77	GLU	N-CA-CB	5.37	120.23	110.08
1	A	372	TYR	CA-CB-CG	5.37	123.56	113.90
1	A	33	PHE	CA-CB-CG	-5.37	108.44	113.80
1	A	52	ARG	N-CA-CB	-5.36	102.24	110.12
1	B	73	LYS	CB-CA-C	5.36	119.96	110.85
1	B	77	GLU	CB-CG-CD	5.36	121.70	112.60
1	A	453	ARG	CA-CB-CG	-5.33	103.44	114.10
1	A	424	TYR	CB-CA-C	-5.29	102.54	110.90
1	A	453	ARG	CG-CD-NE	-5.28	100.38	112.00
1	A	494	ASN	CA-CB-CG	-5.26	107.34	112.60
1	B	56	GLU	CB-CG-CD	5.21	121.47	112.60
1	B	247	PRO	N-CD-CG	-5.21	95.38	103.20
1	A	206	THR	CA-CB-OG1	-5.19	101.81	109.60
1	B	10	PHE	CA-CB-CG	-5.19	108.61	113.80
1	B	413	ARG	CA-CB-CG	5.19	124.48	114.10
1	A	381	ARG	CA-CB-CG	5.17	124.43	114.10
1	A	285	GLN	N-CA-CB	-5.16	102.53	110.16
1	B	89	ARG	CA-C-N	5.14	127.42	120.44
1	B	89	ARG	C-N-CA	5.14	127.42	120.44
1	A	412	ASP	CB-CA-C	-5.12	101.89	110.29
1	B	243	ASN	CA-CB-CG	5.12	117.72	112.60
1	A	483	HIS	CA-CB-CG	-5.12	108.68	113.80
1	A	552	TRP	N-CA-C	-5.12	106.30	112.54
1	A	129	LEU	N-CA-CB	5.11	119.19	110.50
1	B	255	ASP	CA-CB-CG	5.11	117.70	112.60
1	A	271	PHE	N-CA-CB	-5.10	103.72	111.21
1	B	263	ASN	CA-C-N	-5.08	115.96	122.26
1	B	263	ASN	C-N-CA	-5.08	115.96	122.26
1	B	369	TYR	CB-CA-C	-5.07	102.38	110.79
1	B	387	PHE	N-CA-CB	5.06	117.56	110.12
1	B	236	ARG	CD-NE-CZ	5.05	131.48	124.40
1	A	578	THR	CA-CB-OG1	-5.04	102.04	109.60
1	A	417	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	423	ASN	CA-CB-CG	5.02	117.62	112.60
1	B	509	PHE	CA-CB-CG	-5.02	108.78	113.80

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	235[A]	ARG	Sidechain
1	A	235[B]	ARG	Sidechain
1	A	541	ARG	Sidechain
1	A	90	ARG	Sidechain
1	B	120	ARG	Sidechain
1	B	326	ARG	Sidechain
1	B	467	ARG	Sidechain
1	B	541	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	5023	0	4791	43	0
1	B	4987	0	4767	45	0
2	F	24	0	22	6	0
3	A	33	0	0	0	0
3	B	33	0	0	0	0
4	A	21	0	30	0	0
4	B	14	0	20	1	0
5	A	8	0	12	1	0
5	B	12	0	18	4	0
6	A	30	0	42	8	0
6	B	10	0	14	1	0
7	A	19	0	26	4	0
8	A	56	0	52	7	0
8	B	70	0	65	16	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	B	32	0	44	5	0
12	B	13	0	18	4	0
13	B	10	0	10	3	0
14	A	306	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	B	353	0	0	7	0
All	All	11058	0	9931	115	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 (115) 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:B:45:ASN:HD21	8:B:811:NAG:C1	0.91	1.55
1:B:45:ASN:ND2	8:B:811:NAG:C1	1.74	1.40
8:B:811:NAG:O4	8:B:812:NAG:C1	1.74	1.33
8:B:816:NAG:O4	8:B:817:NAG:C1	1.85	1.22
1:B:235:ARG:HH11	12:B:804:PG4:H31	1.26	1.00
8:A:811:NAG:C1	2:F:1:NAG:O4	2.14	0.94
1:B:45:ASN:HD21	8:B:811:NAG:C2	1.83	0.89
1:B:45:ASN:CG	8:B:811:NAG:C1	2.52	0.81
1:A:418:THR:HG23	2:F:2:FUC:O4	1.81	0.80
1:B:477:VAL:HG12	1:B:603:LEU:HD21	1.62	0.79
8:B:816:NAG:O6	13:B:818:FUC:H3	1.83	0.79
1:B:231:ARG:HG3	12:B:804:PG4:H32	1.66	0.76
1:B:155:MET:HA	1:B:155:MET:HE2	1.70	0.74
1:A:418:THR:CG2	2:F:2:FUC:O4	2.36	0.73
6:A:810:PGE:H52	14:A:1175:HOH:O	1.89	0.72
1:B:45:ASN:ND2	8:B:811:NAG:C2	2.47	0.71
8:B:811:NAG:C4	8:B:812:NAG:C1	2.68	0.70
1:B:157:LEU:HD11	1:B:477:VAL:HG13	1.74	0.70
1:A:25:GLN:OE1	1:A:376:PRO:HB2	1.92	0.70
5:B:809:EDO:H11	14:B:1093:HOH:O	1.92	0.69
1:A:292:HIS:NE2	6:A:807:PGE:H3	2.08	0.68
1:B:354:ASP:O	1:B:357[B]:SER:HB3	1.93	0.68
1:B:117:GLN:HG2	14:B:964:HOH:O	1.94	0.67
1:A:292:HIS:CD2	6:A:807:PGE:H3	2.29	0.67
1:B:390:ALA:O	1:B:394:VAL:HG23	1.96	0.66
8:A:811:NAG:H82	2:F:1:NAG:H62	1.80	0.63
8:B:816:NAG:HO6	13:B:818:FUC:H3	1.62	0.63
1:B:83:PHE:HB2	1:B:89:ARG:HG2	1.79	0.63
6:A:810:PGE:H42	14:A:1175:HOH:O	1.99	0.62
8:B:816:NAG:C4	8:B:817:NAG:C1	2.77	0.62
1:B:148:ALA:O	1:B:151[B]:ARG:NH2	2.32	0.62
8:A:815:NAG:O3	8:A:816:NAG:C1	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ALA:O	1:A:394:VAL:HG23	2.00	0.61
1:A:141:PRO:HB3	1:A:350:ARG:HD3	1.83	0.60
6:B:806:PGE:H2	14:B:1216:HOH:O	2.01	0.60
1:B:235:ARG:NH1	12:B:804:PG4:H31	2.08	0.60
1:A:265:TYR:CE1	1:A:427:LYS:HB2	2.37	0.59
1:B:381:ARG:HD3	11:B:802:1PE:H221	1.84	0.59
1:A:80:TRP:O	1:A:89:ARG:HG2	2.03	0.59
1:B:87:GLN:O	1:B:90:ARG:HB2	2.04	0.58
1:A:274:LYS:HE3	1:A:419:GLU:HB2	1.86	0.57
11:B:802:1PE:H222	14:B:1158:HOH:O	2.04	0.57
1:A:49:GLU:HG3	1:A:53:ARG:NH1	2.19	0.57
1:A:513:GLU:HA	1:A:525:LEU:HD11	1.86	0.57
1:A:264:ILE:HB	1:A:267:MET:HE3	1.86	0.56
5:B:809:EDO:C1	14:B:1093:HOH:O	2.52	0.56
1:A:274:LYS:HB3	1:A:275:PRO:CD	2.36	0.55
1:B:45:ASN:ND2	8:B:811:NAG:O5	2.27	0.54
1:B:70:GLN:HE21	1:B:70:GLN:HA	1.73	0.53
8:B:811:NAG:O4	8:B:812:NAG:C2	2.52	0.53
1:A:292:HIS:HE2	6:A:807:PGE:C5	2.22	0.52
1:B:381:ARG:HH11	11:B:802:1PE:H231	1.75	0.52
8:B:816:NAG:O6	13:B:818:FUC:C3	2.55	0.52
1:B:9:GLN:HE22	1:B:71:LYS:NZ	2.07	0.52
1:B:9:GLN:HE22	1:B:71:LYS:HZ2	1.57	0.52
1:A:172:LYS:O	1:A:176[A]:GLU:HG3	2.10	0.51
1:A:236[B]:ARG:NH1	1:A:267:MET:HG2	2.26	0.51
1:B:172:LYS:HB3	1:B:173:PRO:HD3	1.92	0.51
1:A:568:GLN:HB2	1:A:569:PRO:HD3	1.92	0.51
1:A:3:PRO:HA	1:A:6:GLN:HG3	1.91	0.51
7:A:808:P6G:H171	14:A:1174:HOH:O	2.10	0.50
8:A:815:NAG:C3	8:A:816:NAG:C1	2.90	0.50
8:A:815:NAG:H4	8:A:816:NAG:N2	2.26	0.50
1:B:580:TRP:O	1:B:584:GLN:HG2	2.12	0.50
5:B:809:EDO:H21	14:B:1211:HOH:O	2.13	0.49
1:B:510:GLN:HG2	1:B:569:PRO:HG2	1.95	0.49
1:A:157:LEU:HD11	1:A:477:VAL:HG13	1.95	0.48
7:A:808:P6G:H171	7:A:808:P6G:H141	1.55	0.48
1:B:570:LEU:C	1:B:570:LEU:HD23	2.38	0.48
7:A:808:P6G:H141	14:A:1174:HOH:O	2.14	0.47
6:A:810:PGE:H4	14:A:902:HOH:O	2.13	0.47
1:A:389:GLU:HB2	1:A:504[A]:SER:HB2	1.95	0.47
1:B:35:SER:OG	11:B:810:1PE:H152	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:ARG:HG3	7:A:808:P6G:H32	1.96	0.47
1:A:172:LYS:HB3	1:A:173:PRO:HD3	1.97	0.47
1:A:477:VAL:HG12	1:A:603:LEU:HD21	1.96	0.47
1:A:607:TYR:HA	1:A:608:PRO:HA	1.78	0.47
1:B:389:GLU:HB2	1:B:504[B]:SER:HB3	1.97	0.47
1:A:279:VAL:O	1:A:280:THR:C	2.59	0.46
1:A:453:ARG:HH12	6:A:810:PGE:C4	2.29	0.46
1:A:274:LYS:HB3	1:A:275:PRO:HD2	1.97	0.46
1:A:275:PRO:HG2	1:A:414:VAL:HG13	1.97	0.46
11:B:810:1PE:H252	11:B:810:1PE:H262	1.54	0.46
1:A:172:LYS:HB3	1:A:173:PRO:CD	2.46	0.45
1:B:151[A]:ARG:NE	1:B:267:MET:HE2	2.31	0.45
1:B:83:PHE:O	1:B:89:ARG:HD3	2.16	0.45
8:A:811:NAG:N2	2:F:1:NAG:O4	2.50	0.45
1:A:578:THR:O	1:A:582:GLN:HG3	2.17	0.44
1:B:389:GLU:HB2	1:B:504[A]:SER:HB2	1.98	0.44
1:A:441:LEU:HD12	1:A:441:LEU:C	2.42	0.44
8:A:815:NAG:H4	8:A:816:NAG:C1	2.47	0.44
1:B:31:VAL:HG21	1:B:64:PHE:CD1	2.54	0.43
1:B:557:LYS:HE3	14:B:1157:HOH:O	2.19	0.43
1:B:269:VAL:O	1:B:269:VAL:HG13	2.19	0.43
1:B:548:SER:HB2	5:B:805:EDO:H22	1.99	0.43
1:A:596:GLU:OE2	8:B:815:NAG:O7	2.37	0.42
1:A:44:THR:O	1:A:45:ASN:HB2	2.19	0.42
1:A:531:TYR:O	1:A:532:ARG:HB2	2.19	0.42
1:A:236[A]:ARG:O	1:A:236[A]:ARG:HG3	2.19	0.42
1:A:570:LEU:C	1:A:570:LEU:HD23	2.45	0.42
1:B:84:THR:O	1:B:86:PRO:HD3	2.20	0.42
1:B:231:ARG:CG	12:B:804:PG4:H32	2.44	0.42
1:A:243:ASN:HD22	1:A:599:TRP:CG	2.39	0.41
1:B:24:TYR:CE2	1:B:95:VAL:HG22	2.55	0.41
1:B:70:GLN:HA	1:B:70:GLN:NE2	2.36	0.41
1:B:45:ASN:OD1	8:B:811:NAG:C1	2.68	0.41
1:A:30:GLN:HA	5:A:809:EDO:H22	2.02	0.41
1:A:292:HIS:HE2	6:A:807:PGE:H6	1.85	0.41
1:B:334:ALA:C	1:B:335:TRP:CD1	2.98	0.41
1:B:489:LYS:O	1:B:493:PRO:HD2	2.21	0.41
1:A:568:GLN:N	1:A:569:PRO:CD	2.84	0.40
1:A:572:LYS:HA	1:A:575:GLN:HG3	2.03	0.40
1:B:115:LEU:CD2	1:B:495:VAL:HG21	2.52	0.40
1:A:418:THR:HG22	2:F:2:FUC:O4	2.18	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:PHE:CE1	4:B:803:PEG:H21	2.57	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	612/628 (98%)	600 (98%)	10 (2%)	2 (0%)	36	29
1	B	606/628 (96%)	593 (98%)	12 (2%)	1 (0%)	43	36
All	All	1218/1256 (97%)	1193 (98%)	22 (2%)	3 (0%)	36	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	413	ARG
1	A	45	ASN
1	B	45	ASN

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	532/540 (98%)	517 (97%)	15 (3%)	38	32
1	B	526/540 (97%)	514 (98%)	12 (2%)	44	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1058/1080 (98%)	1031 (97%)	27 (3%)	40 35

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	SER
1	A	54	GLN
1	A	74	GLU
1	A	79	ILE
1	A	84	THR
1	A	96	ARG
1	A	129	LEU
1	A	368	TYR
1	A	372	TYR
1	A	381	ARG
1	A	418	THR
1	A	426	LEU
1	A	441	LEU
1	A	453	ARG
1	A	605	ASP
1	B	92	ILE
1	B	96	ARG
1	B	97	THR
1	B	129	LEU
1	B	135	THR
1	B	141	PRO
1	B	155	MET
1	B	268	VAL
1	B	372	TYR
1	B	377	VAL
1	B	388	HIS
1	B	414	VAL

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

Mol	Chain	Res	Type
1	A	213	HIS
1	A	371	GLN
1	A	444	GLN
1	A	588	ASN
1	B	9	GLN

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Mol	Chain	Res	Type
1	B	45	ASN
1	B	70	GLN
1	B	203	ASN
1	B	263	ASN
1	B	371	GLN
1	B	527	GLN
1	B	588	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 ⓘ

2 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	F	1	2,1	14,14,15	0.49	0	17,19,21	1.42	4 (23%)
2	FUC	F	2	2	10,10,11	0.45	0	14,14,16	1.17	1 (7%)

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	F	1	2,1	-	0/6/23/26	0/1/1/1
2	FUC	F	2	2	-	-	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	O3-C3-C2	3.14	115.91	109.40
2	F	1	NAG	C1-O5-C5	2.86	116.02	112.19
2	F	2	FUC	O2-C2-C3	2.77	115.89	110.15
2	F	1	NAG	O4-C4-C3	-2.63	104.19	110.38
2	F	1	NAG	C2-N2-C7	2.49	126.24	122.90

There are no chirality outliers.

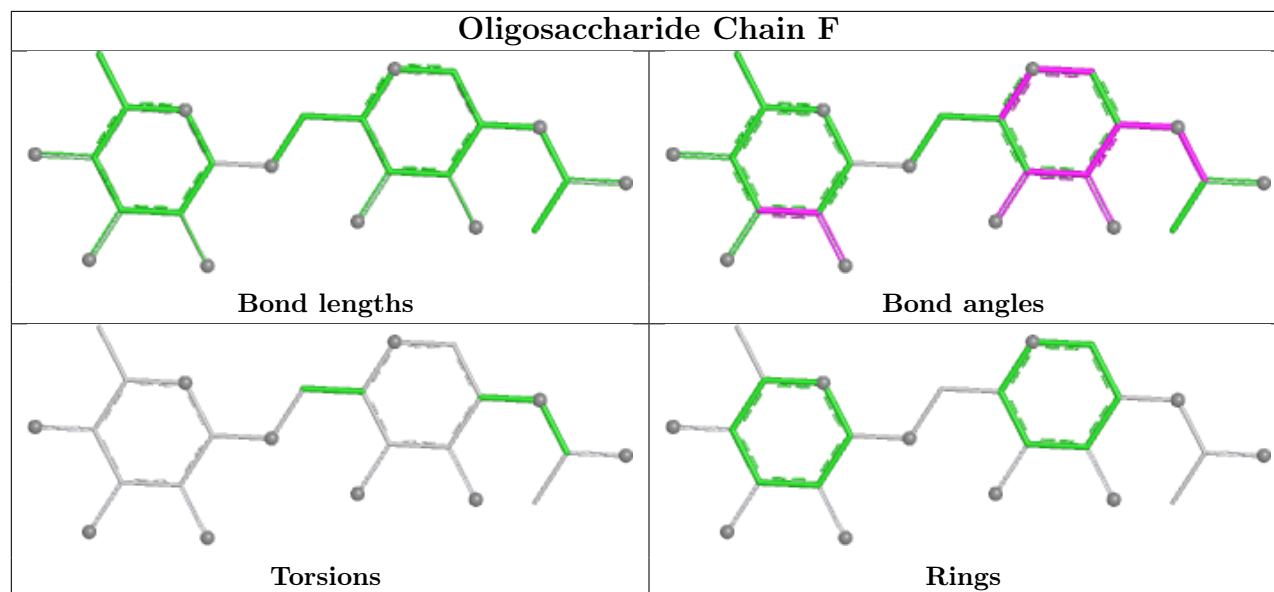
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	FUC	3	0
2	F	1	NAG	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 oligosaccharide.



5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 4 are monoatomic - leaving 30 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	EDO	B	808	-	3,3,3	0.42	0	2,2,2	0.90	0
5	EDO	A	809	-	3,3,3	0.25	0	2,2,2	0.17	0
5	EDO	B	809	-	3,3,3	0.22	0	2,2,2	0.45	0
3	A1IJY	A	801	9	35,35,35	2.95	15 (42%)	44,50,50	2.68	20 (45%)
4	PEG	A	804	-	6,6,6	0.18	0	5,5,5	0.06	0
11	1PE	B	802	-	15,15,15	0.56	0	14,14,14	0.67	0
5	EDO	A	803	-	3,3,3	0.05	0	2,2,2	0.58	0
8	NAG	B	812	-	14,14,15	0.50	0	17,19,21	1.06	2 (11%)
6	PGE	B	806	-	9,9,9	0.32	0	8,8,8	0.25	0
8	NAG	A	815	1	14,14,15	0.52	0	17,19,21	1.69	7 (41%)
8	NAG	B	815	1	14,14,15	0.49	0	17,19,21	1.41	3 (17%)
8	NAG	A	811	-	14,14,15	0.55	0	17,19,21	1.94	5 (29%)
4	PEG	B	803	-	6,6,6	0.19	0	5,5,5	0.18	0
6	PGE	A	806	-	9,9,9	0.29	0	8,8,8	0.26	0
4	PEG	A	802	-	6,6,6	0.67	0	5,5,5	0.59	0
12	PG4	B	804	-	12,12,12	0.26	0	11,11,11	0.36	0
6	PGE	A	810	-	9,9,9	0.23	0	8,8,8	0.26	0
3	A1IJY	B	801	9	35,35,35	3.14	15 (42%)	44,50,50	2.49	23 (52%)
8	NAG	A	814	1	14,14,15	0.51	0	17,19,21	4.09	7 (41%)
7	P6G	A	808	-	18,18,18	0.42	0	17,17,17	0.54	0
11	1PE	B	810	-	15,15,15	0.45	0	14,14,14	0.53	0
4	PEG	A	805	-	6,6,6	0.26	0	5,5,5	0.36	0
8	NAG	B	816	1	14,14,15	0.58	0	17,19,21	1.73	4 (23%)
8	NAG	B	811	-	14,14,15	0.53	0	17,19,21	1.34	3 (17%)
5	EDO	B	805	-	3,3,3	0.94	0	2,2,2	1.06	0
8	NAG	A	816	-	14,14,15	0.43	0	17,19,21	0.72	0
13	FUC	B	818	-	10,10,11	0.61	0	14,14,16	1.13	1 (7%)
6	PGE	A	807	-	9,9,9	0.82	0	8,8,8	0.87	0
4	PEG	B	807	-	6,6,6	0.29	0	5,5,5	0.13	0
8	NAG	B	817	-	14,14,15	0.50	0	17,19,21	1.52	3 (17%)

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	EDO	B	808	-	-	0/1/1/1	-
5	EDO	A	809	-	-	1/1/1/1	-
5	EDO	B	809	-	-	1/1/1/1	-
3	A1IJY	A	801	9	-	6/36/56/56	0/3/3/3
4	PEG	A	804	-	-	1/4/4/4	-
11	1PE	B	802	-	-	7/13/13/13	-
5	EDO	A	803	-	-	0/1/1/1	-
8	NAG	B	812	-	-	2/6/23/26	0/1/1/1
6	PGE	B	806	-	-	4/7/7/7	-
8	NAG	A	815	1	-	2/6/23/26	0/1/1/1
8	NAG	B	815	1	-	2/6/23/26	0/1/1/1
8	NAG	A	811	-	-	2/6/23/26	0/1/1/1
4	PEG	B	803	-	-	4/4/4/4	-
6	PGE	A	806	-	-	6/7/7/7	-
4	PEG	A	802	-	-	3/4/4/4	-
12	PG4	B	804	-	-	7/10/10/10	-
6	PGE	A	810	-	-	4/7/7/7	-
3	A1IJY	B	801	9	-	7/36/56/56	0/3/3/3
8	NAG	A	814	1	-	2/6/23/26	0/1/1/1
7	P6G	A	808	-	-	9/16/16/16	-
11	1PE	B	810	-	-	6/13/13/13	-
4	PEG	A	805	-	-	2/4/4/4	-
8	NAG	B	816	1	-	0/6/23/26	0/1/1/1
8	NAG	B	811	-	-	0/6/23/26	0/1/1/1
5	EDO	B	805	-	-	1/1/1/1	-
8	NAG	A	816	-	-	2/6/23/26	0/1/1/1
13	FUC	B	818	-	-	-	0/1/1/1
6	PGE	A	807	-	-	4/7/7/7	-
4	PEG	B	807	-	-	3/4/4/4	-
8	NAG	B	817	-	-	1/6/23/26	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	A1IJY	C06-N10	-9.59	1.35	1.46
3	A	801	A1IJY	C06-N10	-8.68	1.36	1.46
3	A	801	A1IJY	C09-N10	6.92	1.61	1.47
3	A	801	A1IJY	C27-N26	6.69	1.60	1.47
3	B	801	A1IJY	C09-N10	5.97	1.59	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	A1IJY	C27-N26	5.87	1.59	1.47
3	B	801	A1IJY	C13-C12	5.70	1.48	1.39
3	B	801	A1IJY	C07-C06	5.64	1.63	1.53
3	A	801	A1IJY	C30-N26	-4.70	1.37	1.47
3	B	801	A1IJY	C30-N26	-4.44	1.38	1.47
3	A	801	A1IJY	C11-N10	4.40	1.44	1.34
3	B	801	A1IJY	C14-C15	4.00	1.45	1.39
3	A	801	A1IJY	C05-N04	3.70	1.50	1.46
3	A	801	A1IJY	C13-C12	3.32	1.44	1.39
3	A	801	A1IJY	C02-N26	3.10	1.41	1.34
3	B	801	A1IJY	C29-C30	3.07	1.61	1.53
3	B	801	A1IJY	C02-N26	3.05	1.41	1.34
3	B	801	A1IJY	C28-C27	-2.98	1.41	1.51
3	B	801	A1IJY	C11-N10	2.83	1.41	1.34
3	B	801	A1IJY	O24-C22	2.68	1.30	1.22
3	A	801	A1IJY	C07-C06	2.53	1.57	1.53
3	B	801	A1IJY	C08-C07	2.42	1.61	1.51
3	A	801	A1IJY	C30-C31	2.32	1.56	1.52
3	A	801	A1IJY	O01-C02	-2.26	1.18	1.22
3	A	801	A1IJY	C28-C29	2.18	1.60	1.51
3	A	801	A1IJY	C05-C22	2.14	1.55	1.52
3	A	801	A1IJY	O21-C11	-2.13	1.18	1.22
3	B	801	A1IJY	C08-C09	-2.11	1.44	1.51
3	B	801	A1IJY	C20-C19	2.10	1.42	1.38
3	A	801	A1IJY	C28-C27	-2.03	1.44	1.51

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	814	NAG	C2-N2-C7	-14.44	103.55	122.90
3	A	801	A1IJY	C19-C20-C12	-6.36	114.01	120.80
3	A	801	A1IJY	O23-C22-O24	-6.30	109.79	124.08
3	B	801	A1IJY	C14-C13-C12	-6.23	114.15	120.80
3	A	801	A1IJY	C13-C14-C15	-5.96	114.43	120.80
3	A	801	A1IJY	O23-C22-C05	5.52	133.31	114.15
3	B	801	A1IJY	C19-C15-C14	4.68	124.52	118.57
3	B	801	A1IJY	C20-C12-C13	4.63	124.46	118.57
8	A	811	NAG	C2-N2-C7	4.47	128.89	122.90
8	B	816	NAG	C1-C2-N2	4.26	117.15	110.43
3	B	801	A1IJY	C09-N10-C06	4.21	118.33	111.69
8	A	814	NAG	O3-C3-C2	-4.21	100.65	109.40
8	B	817	NAG	C2-N2-C7	4.18	128.50	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	814	NAG	C1-O5-C5	4.10	117.68	112.19
3	B	801	A1IJY	O32-C31-O33	-4.06	114.86	124.08
3	B	801	A1IJY	O01-C02-N26	-4.05	114.11	121.38
3	B	801	A1IJY	O23-C22-O24	-3.89	115.25	124.08
3	A	801	A1IJY	O21-C11-N10	-3.72	115.65	121.62
3	A	801	A1IJY	C08-C07-C06	-3.59	98.21	104.21
3	A	801	A1IJY	C20-C19-C15	3.57	124.62	120.80
8	A	814	NAG	O5-C1-C2	3.47	116.67	111.29
3	A	801	A1IJY	C08-C09-N10	-3.44	97.32	103.24
8	A	811	NAG	O5-C1-C2	3.38	116.52	111.29
8	A	811	NAG	C1-C2-N2	3.36	115.73	110.43
3	A	801	A1IJY	C31-C30-N26	-3.30	105.92	112.54
3	A	801	A1IJY	C03-C02-N26	3.29	124.60	118.09
3	B	801	A1IJY	C20-C19-C15	-3.23	117.35	120.80
3	B	801	A1IJY	O32-C31-C30	3.13	123.55	113.34
8	B	816	NAG	O4-C4-C3	-3.13	103.00	110.38
3	A	801	A1IJY	C19-C15-C14	3.11	122.52	118.57
3	B	801	A1IJY	O23-C22-C05	3.09	124.86	114.15
3	A	801	A1IJY	O32-C31-O33	-3.07	117.12	124.08
3	B	801	A1IJY	O17-C16-C15	-3.04	113.50	121.46
3	A	801	A1IJY	C28-C27-N26	3.01	108.42	103.24
8	A	815	NAG	C1-O5-C5	-2.96	108.22	112.19
8	B	815	NAG	O3-C3-C2	-2.95	103.27	109.40
8	A	814	NAG	C4-C3-C2	2.93	115.31	111.02
8	A	811	NAG	O3-C3-C2	-2.89	103.40	109.40
8	B	811	NAG	O5-C1-C2	-2.88	106.84	111.29
8	B	817	NAG	O5-C1-C2	2.84	115.68	111.29
3	A	801	A1IJY	C29-C30-N26	2.82	107.16	103.02
8	A	811	NAG	C1-O5-C5	2.80	115.94	112.19
3	A	801	A1IJY	O01-C02-N26	-2.80	116.36	121.38
3	B	801	A1IJY	O18-C16-C15	2.74	121.88	114.84
3	B	801	A1IJY	O21-C11-N10	-2.71	117.27	121.62
3	A	801	A1IJY	O32-C31-C30	2.70	122.14	113.34
3	B	801	A1IJY	C07-C06-N10	-2.66	100.43	102.66
8	B	811	NAG	C1-C2-N2	2.66	114.62	110.43
3	A	801	A1IJY	C20-C12-C13	2.62	121.90	118.57
8	A	815	NAG	C4-C3-C2	2.58	114.79	111.02
8	A	815	NAG	O5-C1-C2	-2.56	107.32	111.29
3	B	801	A1IJY	C29-C30-C31	-2.54	105.86	111.26
8	A	814	NAG	O7-C7-N2	-2.53	117.50	121.98
8	B	811	NAG	C2-N2-C7	2.51	126.27	122.90
8	B	815	NAG	C1-O5-C5	2.48	115.50	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	816	NAG	O5-C1-C2	2.44	115.06	111.29
3	B	801	A1IJY	C29-C30-N26	2.43	106.58	103.02
8	B	817	NAG	O4-C4-C5	2.40	115.23	109.32
8	B	812	NAG	C1-O5-C5	2.27	115.23	112.19
3	A	801	A1IJY	C07-C06-N10	-2.26	100.76	102.66
3	B	801	A1IJY	C08-C09-N10	-2.25	99.36	103.24
3	B	801	A1IJY	C09-N10-C11	-2.25	116.86	125.45
3	A	801	A1IJY	C09-N10-C06	2.24	115.23	111.69
3	B	801	A1IJY	C07-C08-C09	2.24	111.12	104.90
3	B	801	A1IJY	C12-C11-N10	2.23	123.12	118.72
8	B	812	NAG	C1-C2-N2	2.22	113.93	110.43
8	A	815	NAG	C2-N2-C7	-2.15	120.02	122.90
3	B	801	A1IJY	O01-C02-C03	2.14	124.57	120.15
3	B	801	A1IJY	C19-C15-C16	-2.13	116.15	120.37
8	A	814	NAG	C1-C2-N2	2.12	113.77	110.43
8	A	815	NAG	O6-C6-C5	-2.11	104.15	111.33
8	A	815	NAG	O3-C3-C2	-2.11	105.02	109.40
3	B	801	A1IJY	C08-C07-C06	-2.05	100.79	104.21
8	A	815	NAG	C3-C4-C5	2.03	113.92	110.23
3	A	801	A1IJY	C29-C30-C31	-2.03	106.94	111.26
8	B	816	NAG	O5-C5-C4	-2.02	105.90	110.83
8	B	815	NAG	O6-C6-C5	2.01	118.19	111.33
13	B	818	FUC	O2-C2-C3	2.00	114.30	110.15

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	A1IJY	N04-C05-C06-C07
3	B	801	A1IJY	C22-C05-N04-C03
3	B	801	A1IJY	N04-C05-C06-C07
3	B	801	A1IJY	C22-C05-C06-C07
8	A	816	NAG	O7-C7-N2-C2
11	B	810	1PE	C25-C15-OH6-C26
3	B	801	A1IJY	C14-C15-C16-O18
7	A	808	P6G	C14-C15-O16-C17
8	A	816	NAG	C8-C7-N2-C2
6	A	807	PGE	C3-C4-O3-C5
3	A	801	A1IJY	C14-C15-C16-O18
6	B	806	PGE	O1-C1-C2-O2
3	B	801	A1IJY	C19-C15-C16-O18
8	A	815	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	A	811	NAG	O5-C5-C6-O6
3	A	801	A1IJY	C19-C15-C16-O18
3	A	801	A1IJY	C14-C15-C16-O17
12	B	804	PG4	O1-C1-C2-O2
8	A	815	NAG	O5-C5-C6-O6
8	B	815	NAG	O5-C5-C6-O6
7	A	808	P6G	O10-C11-C12-O13
7	A	808	P6G	C11-C12-O13-C14
8	B	812	NAG	C4-C5-C6-O6
3	B	801	A1IJY	C14-C15-C16-O17
8	B	815	NAG	C4-C5-C6-O6
4	A	805	PEG	O1-C1-C2-O2
7	A	808	P6G	O1-C2-C3-O4
7	A	808	P6G	O4-C5-C6-O7
8	A	811	NAG	C4-C5-C6-O6
11	B	810	1PE	C23-C13-OH4-C24
6	A	810	PGE	O2-C3-C4-O3
8	B	812	NAG	O5-C5-C6-O6
6	A	807	PGE	O1-C1-C2-O2
6	A	806	PGE	O2-C3-C4-O3
11	B	802	1PE	C25-C15-OH6-C26
11	B	802	1PE	OH6-C15-C25-OH5
3	A	801	A1IJY	C19-C15-C16-O17
8	A	814	NAG	C4-C5-C6-O6
11	B	802	1PE	OH4-C13-C23-OH3
11	B	802	1PE	OH2-C12-C22-OH3
8	A	814	NAG	O5-C5-C6-O6
4	B	803	PEG	O2-C3-C4-O4
12	B	804	PG4	O4-C7-C8-O5
6	B	806	PGE	C6-C5-O3-C4
7	A	808	P6G	O7-C8-C9-O10
4	B	807	PEG	O1-C1-C2-O2
6	B	806	PGE	O3-C5-C6-O4
11	B	802	1PE	OH7-C16-C26-OH6
3	B	801	A1IJY	C19-C15-C16-O17
5	B	805	EDO	O1-C1-C2-O2
11	B	810	1PE	OH6-C15-C25-OH5
4	A	804	PEG	O1-C1-C2-O2
4	A	805	PEG	O2-C3-C4-O4
11	B	810	1PE	OH5-C14-C24-OH4
6	A	806	PGE	C3-C4-O3-C5
6	A	810	PGE	C6-C5-O3-C4

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Mol	Chain	Res	Type	Atoms
4	B	807	PEG	C1-C2-O2-C3
6	A	806	PGE	C6-C5-O3-C4
6	A	810	PGE	C3-C4-O3-C5
12	B	804	PG4	C3-C4-O3-C5
4	A	802	PEG	O1-C1-C2-O2
4	B	803	PEG	O1-C1-C2-O2
7	A	808	P6G	C5-C6-O7-C8
11	B	802	1PE	C12-C22-OH3-C23
3	A	801	A1IJY	C22-C05-C06-C07
12	B	804	PG4	C4-C3-O2-C2
4	B	803	PEG	C1-C2-O2-C3
6	A	806	PGE	C4-C3-O2-C2
11	B	810	1PE	C12-C22-OH3-C23
4	A	802	PEG	C1-C2-O2-C3
7	A	808	P6G	C18-C17-O16-C15
12	B	804	PG4	C8-C7-O4-C6
11	B	802	1PE	C24-C14-OH5-C25
6	A	810	PGE	O3-C5-C6-O4
6	B	806	PGE	C3-C4-O3-C5
12	B	804	PG4	C6-C5-O3-C4
7	A	808	P6G	O13-C14-C15-O16
5	A	809	EDO	O1-C1-C2-O2
4	B	807	PEG	O2-C3-C4-O4
11	B	810	1PE	C16-C26-OH6-C15
4	B	803	PEG	C4-C3-O2-C2
5	B	809	EDO	O1-C1-C2-O2
4	A	802	PEG	O2-C3-C4-O4
8	B	817	NAG	C4-C5-C6-O6
12	B	804	PG4	O3-C5-C6-O4
6	A	807	PGE	O2-C3-C4-O3
6	A	806	PGE	C1-C2-O2-C3
6	A	807	PGE	C1-C2-O2-C3
6	A	806	PGE	O1-C1-C2-O2

There are no ring outliers.

20 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	809	EDO	1	0
5	B	809	EDO	3	0
11	B	802	1PE	3	0
8	B	812	NAG	3	0

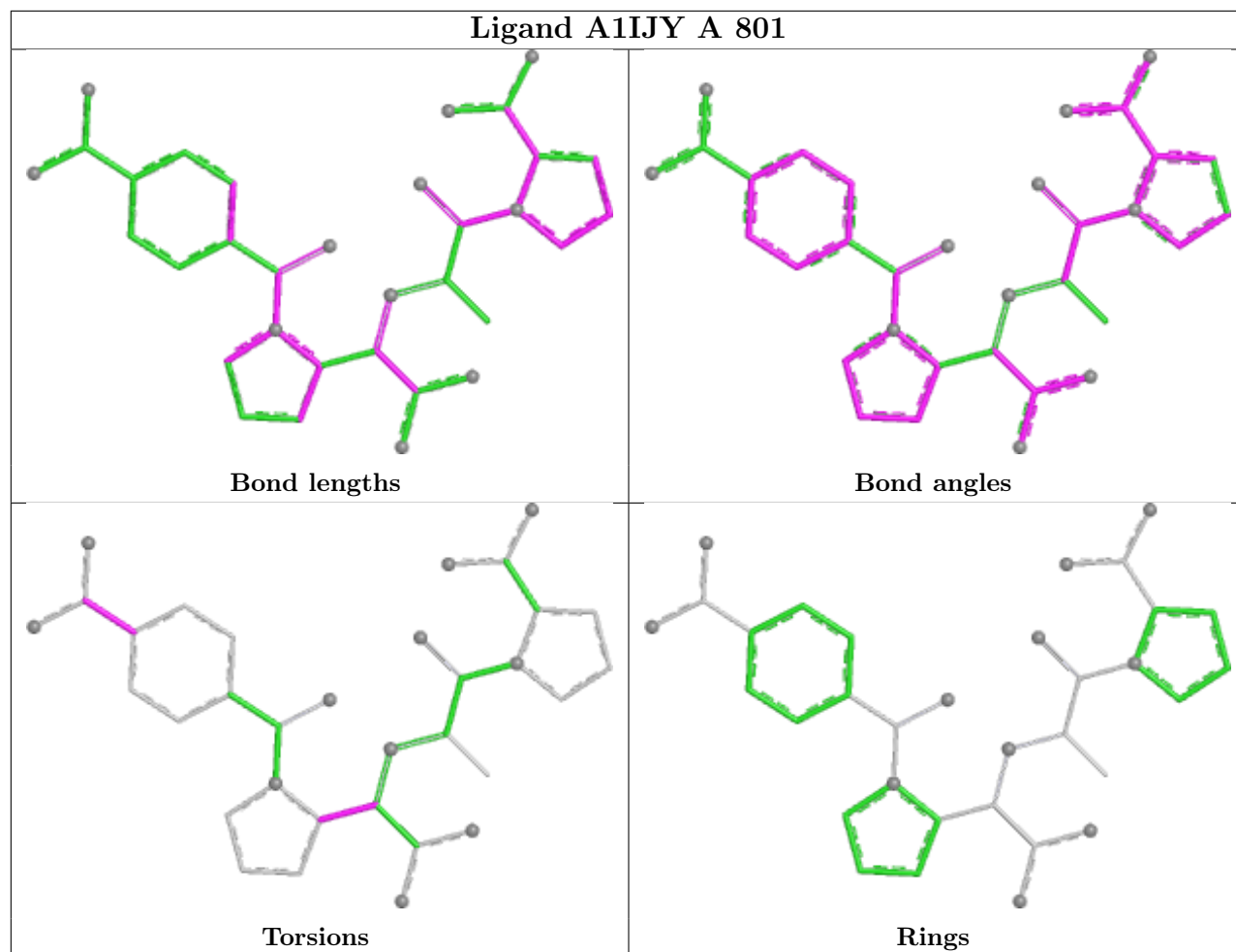
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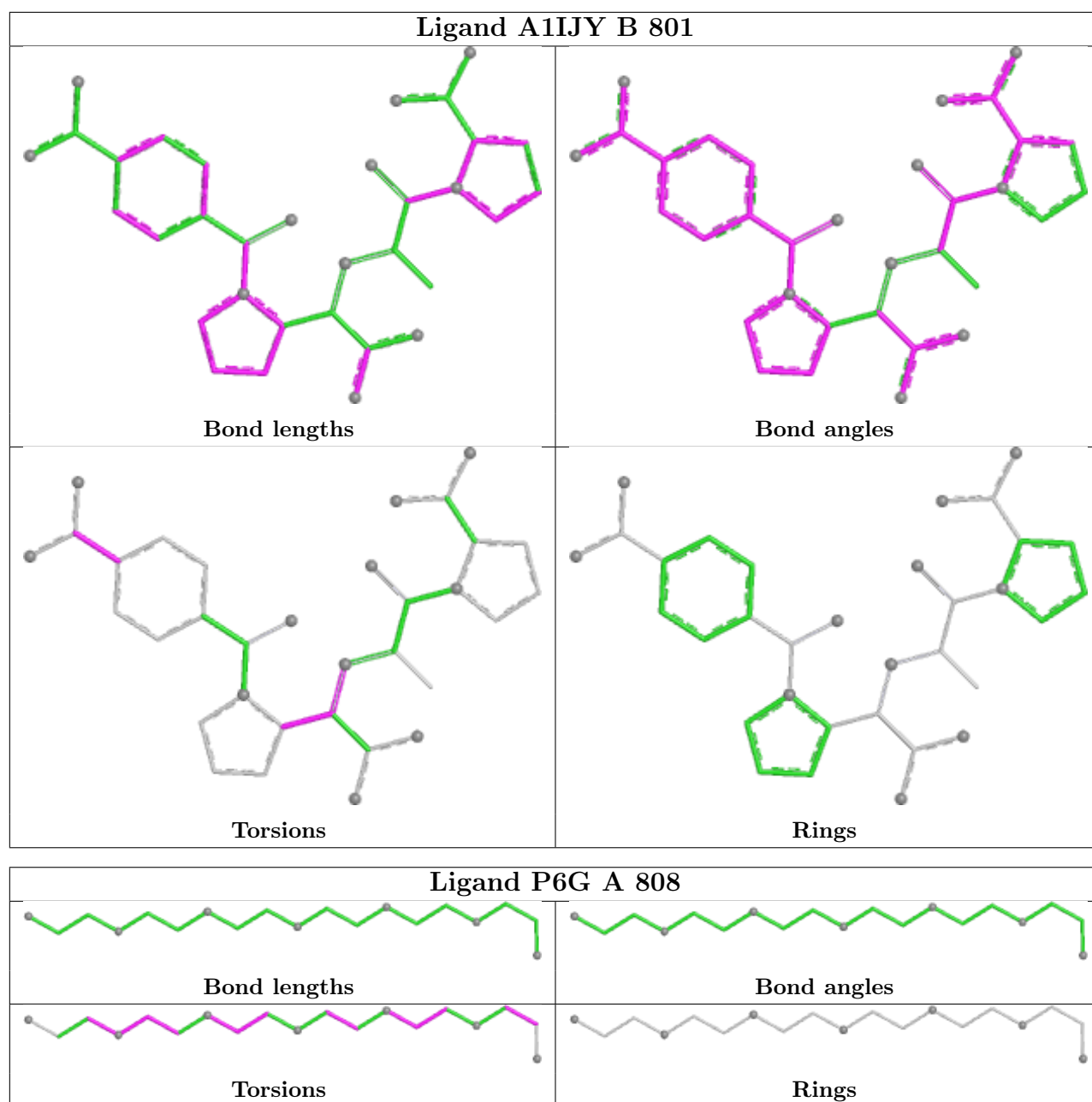
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	806	PGE	1	0
8	A	815	NAG	4	0
8	B	815	NAG	1	0
8	A	811	NAG	3	0
4	B	803	PEG	1	0
12	B	804	PG4	4	0
6	A	810	PGE	4	0
7	A	808	P6G	4	0
11	B	810	1PE	2	0
8	B	816	NAG	5	0
8	B	811	NAG	10	0
5	B	805	EDO	1	0
8	A	816	NAG	4	0
13	B	818	FUC	3	0
6	A	807	PGE	4	0
8	B	817	NAG	2	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 A1IJY A 801





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	603/628 (96%)	-0.24	4 (0%) 84 86	11, 33, 62, 105	13 (2%)
1	B	603/628 (96%)	-0.33	8 (1%) 75 78	9, 30, 54, 99	6 (0%)
All	All	1206/1256 (96%)	-0.28	12 (0%) 79 82	9, 32, 59, 105	19 (1%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	129	LEU	4.7
1	B	129	LEU	4.0
1	B	608	PRO	3.3
1	B	607	TYR	2.8
1	B	135	THR	2.7
1	B	414	VAL	2.7
1	A	135	THR	2.6
1	A	78	PRO	2.5
1	B	262	GLU	2.3
1	B	606	ASN	2.2
1	B	80	TRP	2.1
1	A	236[A]	ARG	2.1

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

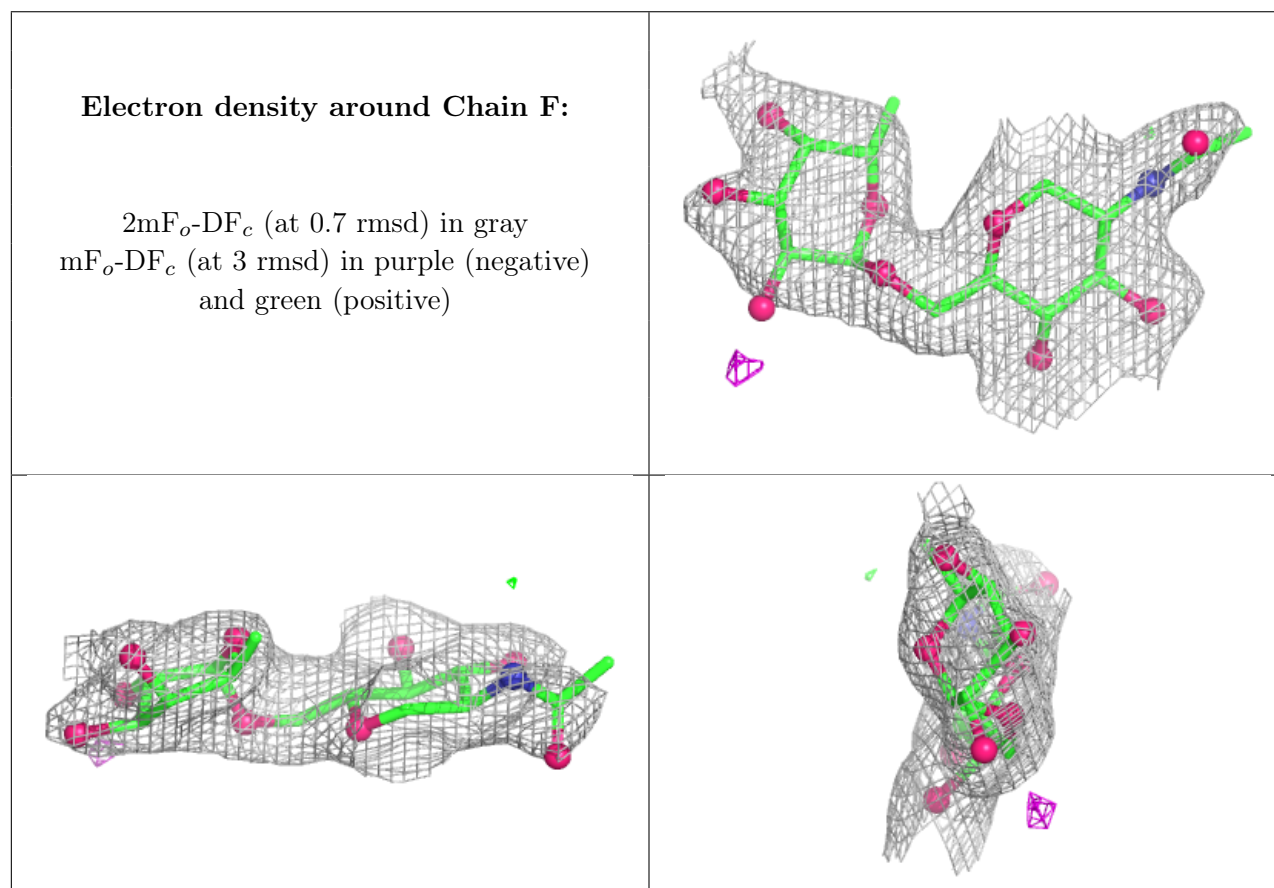
There are no non-standard protein/DNA/RNA residues in this entry.

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, 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
2	NAG	F	1	14/15	-	-	53,61,83,89	0
2	FUC	F	2	10/11	-	-	66,75,81,86	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.



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
8	NAG	A	816	14/15	0.78	0.13	60,105,117,117	0
8	NAG	B	812	14/15	0.79	0.12	41,73,91,95	0
6	PGE	B	806	10/10	0.80	0.16	57,64,74,75	0
5	EDO	B	805	4/4	0.81	0.18	41,62,66,77	0
6	PGE	A	807	10/10	0.83	0.14	37,48,54,57	0
8	NAG	A	811	14/15	0.84	0.12	66,79,86,92	0

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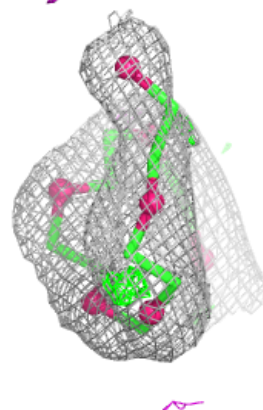
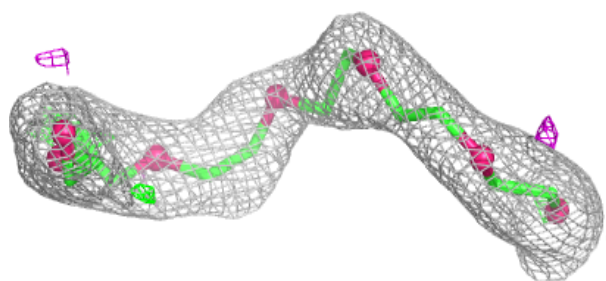
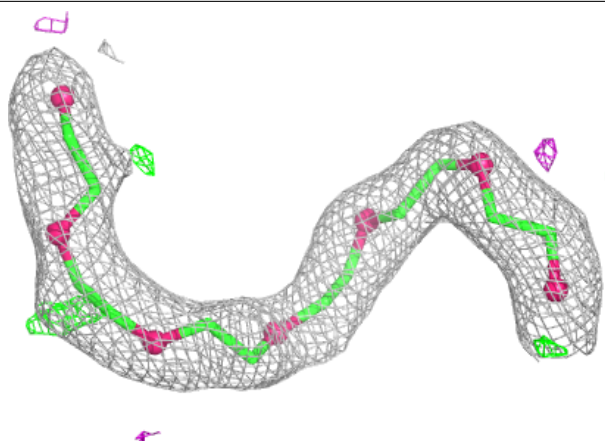
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	NAG	B	817	14/15	0.85	0.11	56,68,78,79	0
8	NAG	A	814	14/15	0.86	0.10	32,48,68,69	0
5	EDO	B	808	4/4	0.86	0.14	63,65,77,79	0
8	NAG	A	815	14/15	0.88	0.11	43,57,84,93	0
12	PG4	B	804	13/13	0.88	0.13	41,60,74,74	0
13	FUC	B	818	10/11	0.88	0.11	59,70,83,92	0
4	PEG	B	807	7/7	0.89	0.12	49,60,74,83	0
5	EDO	B	809	4/4	0.90	0.14	50,61,64,65	0
11	1PE	B	810	16/16	0.90	0.15	42,68,83,92	0
4	PEG	A	804	7/7	0.90	0.14	61,67,69,70	0
8	NAG	B	815	14/15	0.90	0.11	35,46,54,65	0
11	1PE	B	802	16/16	0.91	0.12	39,50,66,68	0
7	P6G	A	808	19/19	0.91	0.12	40,56,70,75	0
8	NAG	B	816	14/15	0.92	0.08	40,48,68,72	0
4	PEG	A	805	7/7	0.92	0.11	46,49,61,67	0
5	EDO	A	803	4/4	0.92	0.10	53,62,62,69	0
8	NAG	B	811	14/15	0.92	0.09	41,48,54,54	0
4	PEG	B	803	7/7	0.92	0.10	54,59,64,67	0
6	PGE	A	810	10/10	0.92	0.10	52,53,72,83	0
6	PGE	A	806	10/10	0.94	0.10	47,58,67,67	0
5	EDO	A	809	4/4	0.94	0.10	55,55,56,59	0
4	PEG	A	802	7/7	0.94	0.09	41,46,53,59	0
3	A1IJY	B	801	33/33	0.97	0.05	17,21,29,33	0
3	A1IJY	A	801	33/33	0.98	0.04	19,24,31,36	0
10	CL	B	814	1/1	0.99	0.03	24,24,24,24	0
10	CL	A	813	1/1	1.00	0.03	26,26,26,26	0
9	ZN	A	812	1/1	1.00	0.01	21,21,21,21	0
9	ZN	B	813	1/1	1.00	0.01	21,21,21,21	0

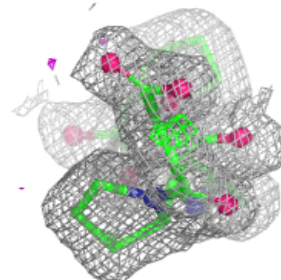
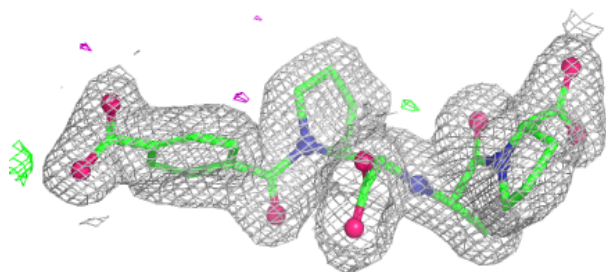
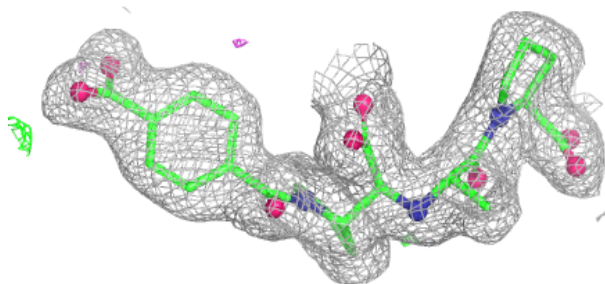
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P6G A 808:

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

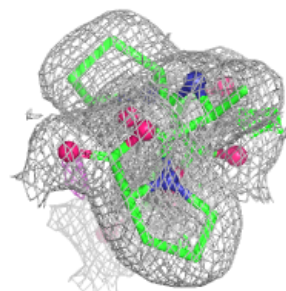
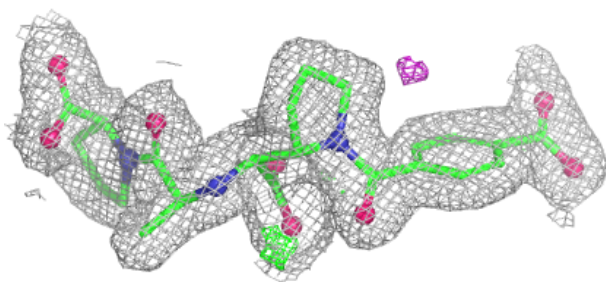
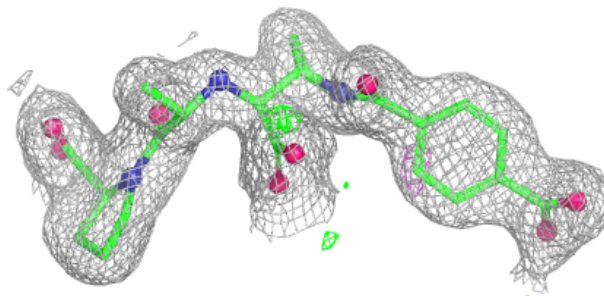
**Electron density around A1IJY B 801:**

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



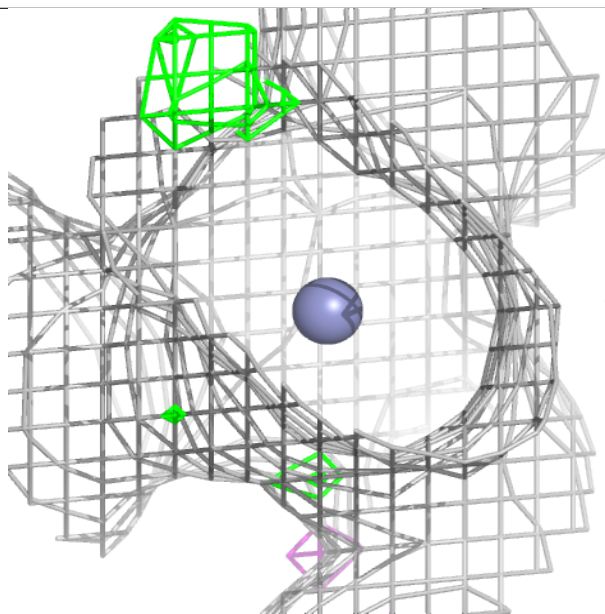
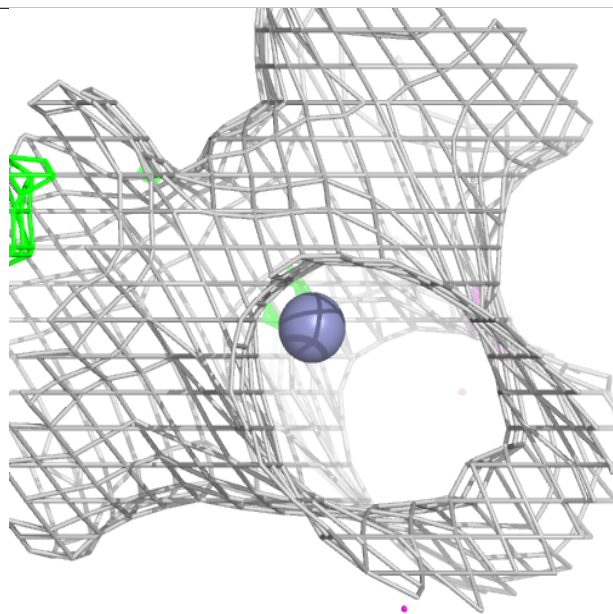
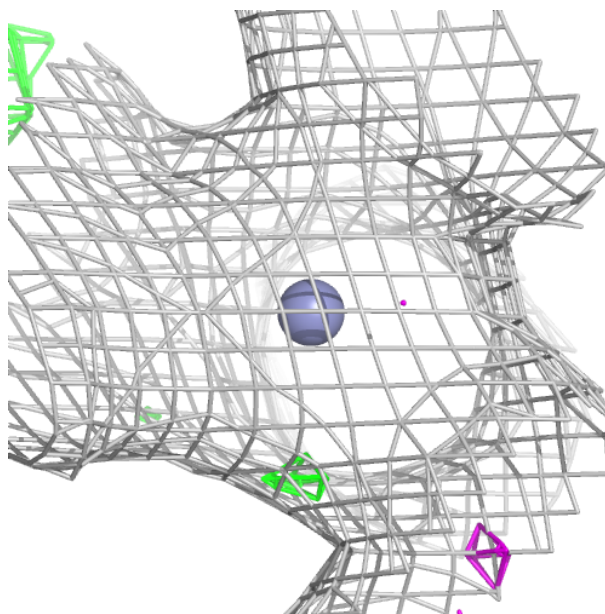
Electron density around A1IJY A 801:

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



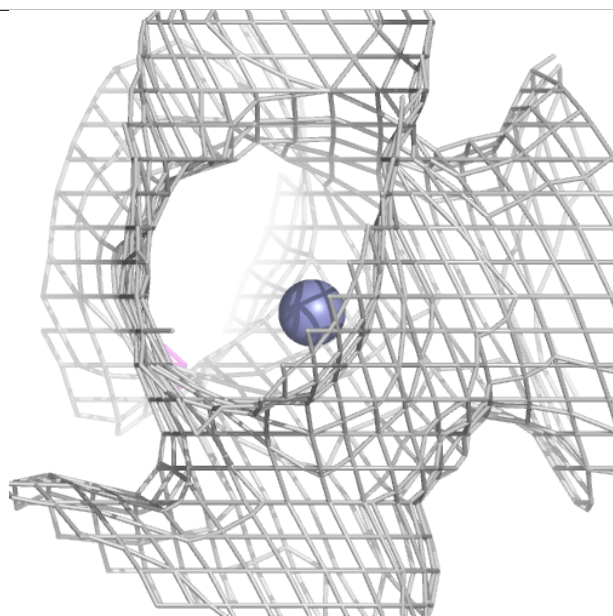
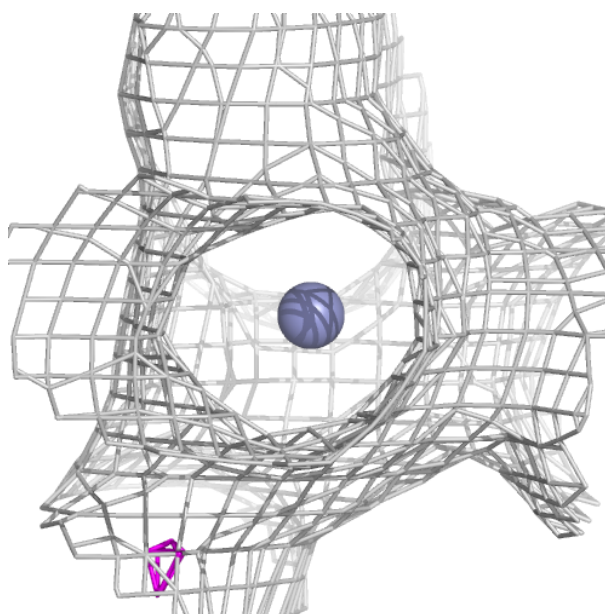
Electron density around ZN A 812:

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



Electron density around ZN B 813:

$2mF_o-DF_c$ (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.