wwPDB X-ray Structure Validation Summary Report (i)

Jan 16, 2025 – 06:47 am GMT

PDB ID	:	9GBS
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 wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

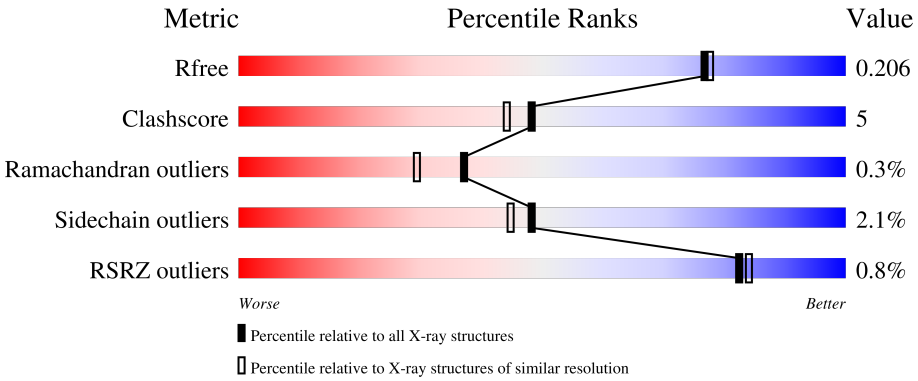
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (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 <=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	84% 10%
1	B	628	% 84% 12%
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 (i)

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			

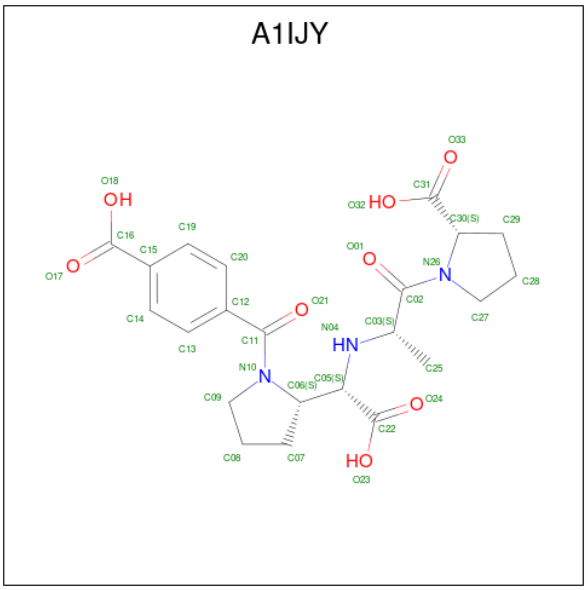
There are 16 discrepancies between the modelled and reference sequences:

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.

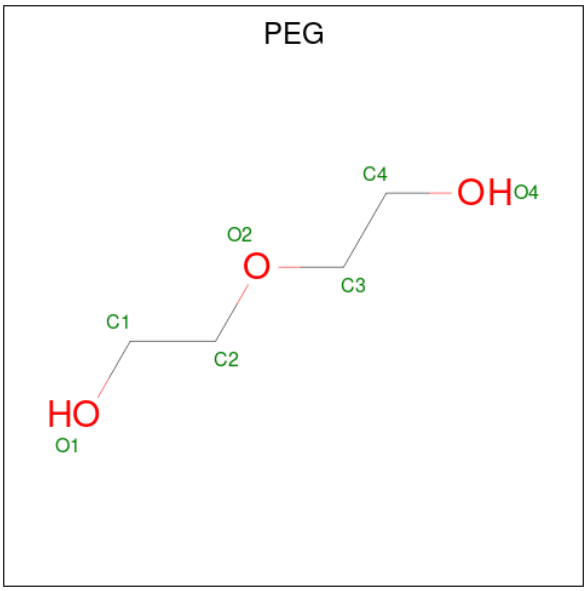
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	F	2	Total C N O 24 14 1 9	0	0	0

- 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 (three-letter code: A1IJY) (formula: $C_{22}H_{27}N_3O_8$).



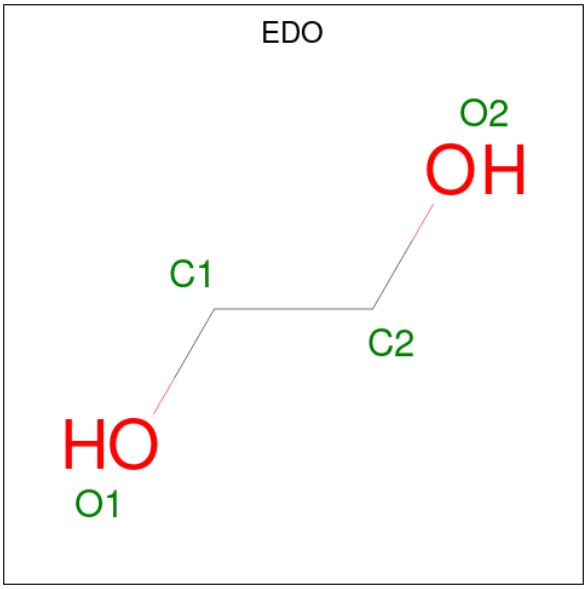
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 33 22 3 8	0	0
3	B	1	Total C N O 33 22 3 8	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



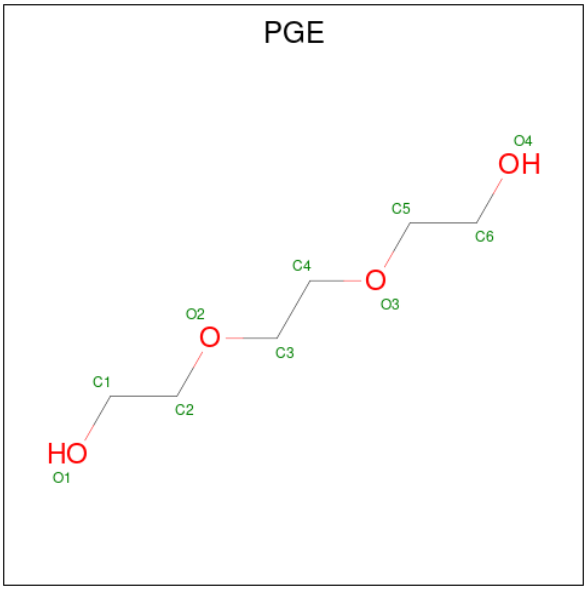
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



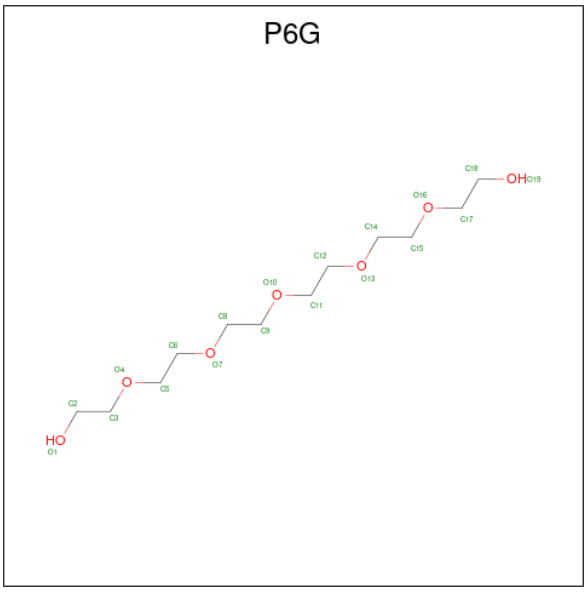
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



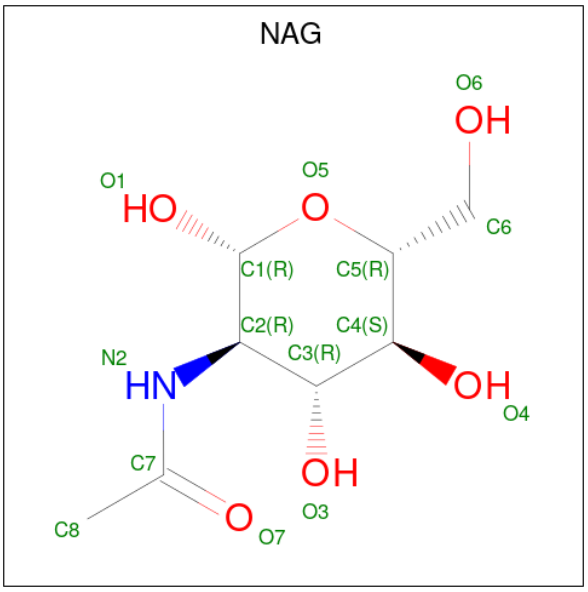
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 10 6 4	0	0
6	A	1	Total C O 10 6 4	0	0
6	A	1	Total C O 10 6 4	0	0
6	B	1	Total C O 10 6 4	0	0

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



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

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

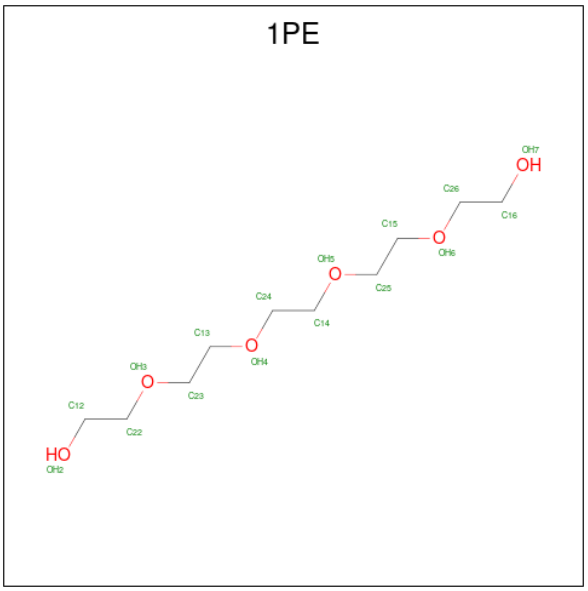
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

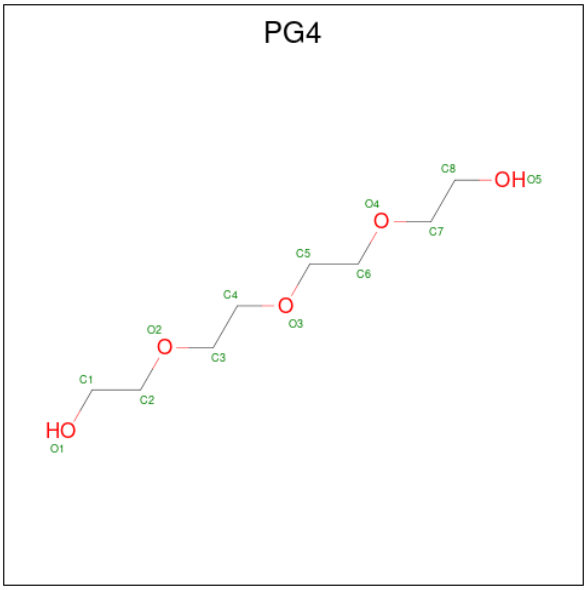
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total Cl 1 1	0	0
10	B	1	Total Cl 1 1	0	0

- Molecule 11 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



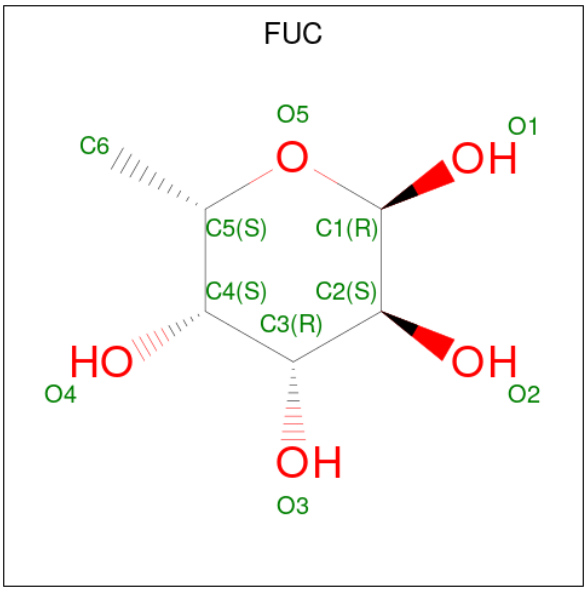
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total C O 16 10 6	0	0
11	B	1	Total C O 16 10 6	0	0

- Molecule 12 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



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

- Molecule 13 is alpha-L-fucopyranose (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



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

- Molecule 14 is water.

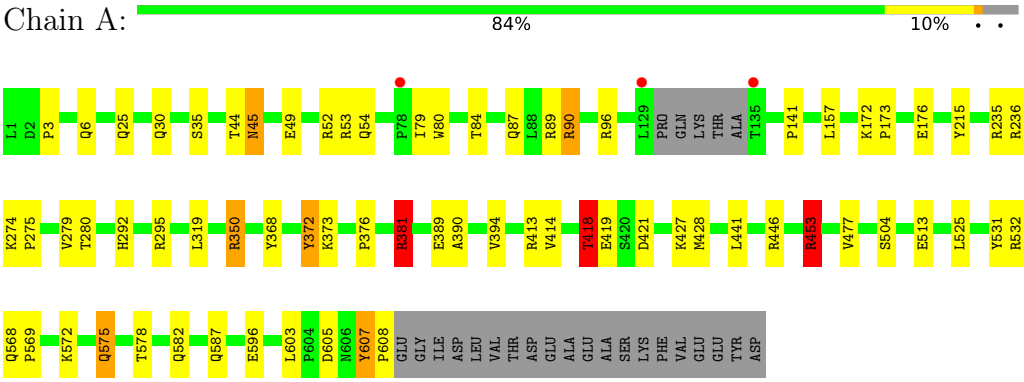
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	306	Total O 306 306	0	0
14	B	353	Total O 353 353	0	0

3 Residue-property plots (i)

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

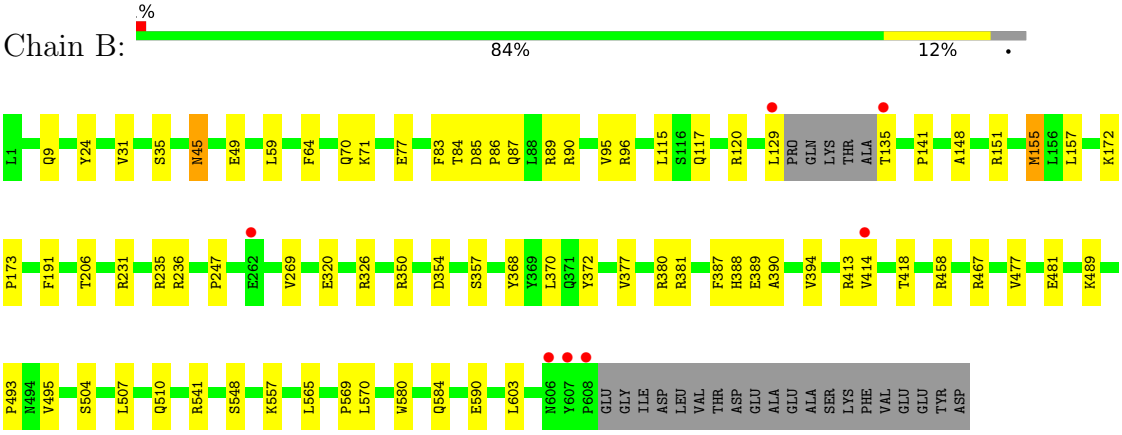
• Molecule 1: Angiotensin-converting enzyme, soluble form

Chain A:



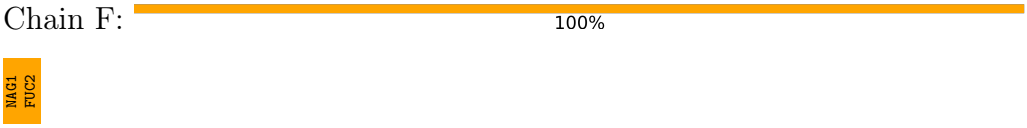
• Molecule 1: Angiotensin-converting enzyme, soluble form

Chain B:



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

Chain F:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	6003 reflections (4.93%)	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]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, NAG, PGE, CL, A1IJY, ZN, FUC, 1PE, PG4, EDO, P6G

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	0.67	0/5181	1.17	23/7054 (0.3%)
1	B	0.73	1/5142 (0.0%)	1.20	23/7001 (0.3%)
All	All	0.70	1/10323 (0.0%)	1.19	46/14055 (0.3%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	481	GLU	CD-OE2	-5.07	1.20	1.25

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	458	ARG	NE-CZ-NH2	-8.13	116.24	120.30
1	A	87	GLN	CB-CA-C	-7.62	95.16	110.40
1	B	350	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	A	52	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	A	52	ARG	CD-NE-CZ	6.58	132.82	123.60

There are no chirality outliers.

5 of 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

5.2 Too-close contacts (i)

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	39	0
1	B	4987	0	4767	44	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	15	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	2	0
14	A	306	0	0	5	0
14	B	353	0	0	7	0
All	All	11058	0	9931	109	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 5.

The worst 5 of 109 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

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%)	37	29
1	B	606/628 (96%)	593 (98%)	12 (2%)	1 (0%)	44	36
All	All	1218/1256 (97%)	1193 (98%)	22 (2%)	3 (0%)	37	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%)	519 (98%)	13 (2%)	44	39
1	B	526/540 (97%)	517 (98%)	9 (2%)	56	54
All	All	1058/1080 (98%)	1036 (98%)	22 (2%)	48	45

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	135	THR
1	B	368	TYR
1	B	155	MET
1	B	372	TYR
1	A	372	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	45	ASN
1	B	70	GLN
1	B	588	ASN
1	B	263	ASN
1	B	9	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	0.47	0	17,19,21	1.41	4 (23%)
2	FUC	F	2	2	10,10,11	0.45	0	14,14,16	1.32	2 (14%)

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.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1	NAG	O3-C3-C2	3.12	115.91	109.47
2	F	2	FUC	O2-C2-C3	2.87	115.89	110.14
2	F	1	NAG	C1-O5-C5	2.83	116.02	112.19
2	F	2	FUC	O5-C1-C2	-2.74	106.54	110.77
2	F	1	NAG	O4-C4-C3	-2.67	104.19	110.35

There are no chirality outliers.

There are no torsion outliers.

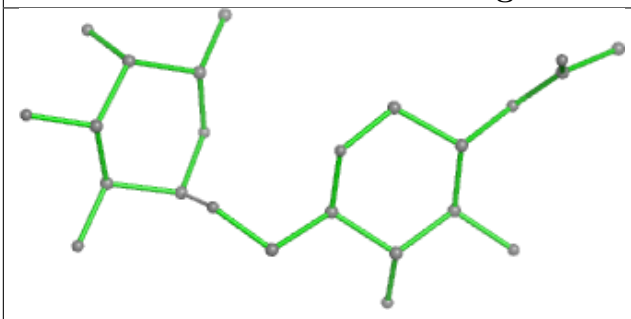
There are no ring outliers.

2 monomers are involved in 6 short contacts:

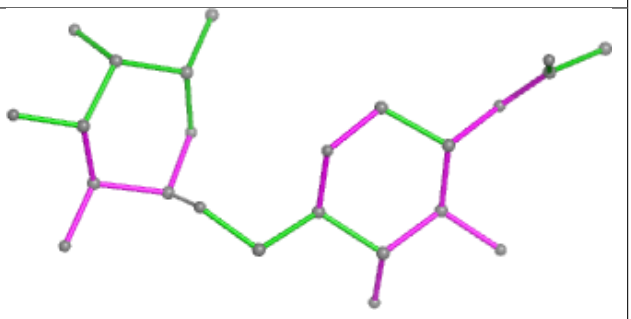
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	FUC	3	0
2	F	1	NAG	3	0

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

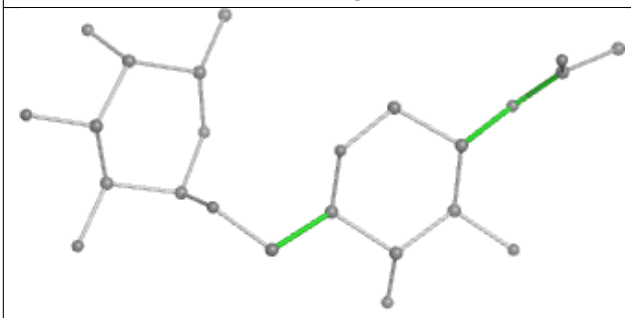
Oligosaccharide Chain F



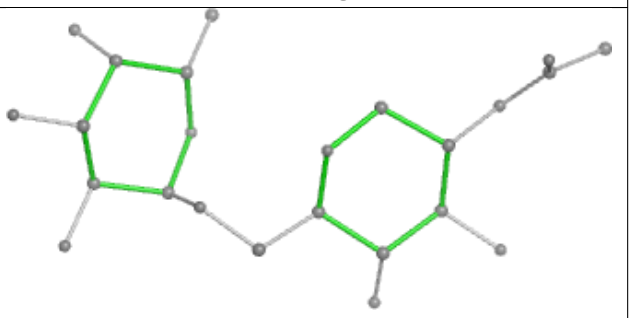
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

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	$\#\|Z\| > 2$
6	PGE	A	807	-	9,9,9	0.82	0	8,8,8	0.88	0
8	NAG	A	811	-	14,14,15	0.53	0	17,19,21	1.87	5 (29%)
8	NAG	B	815	1	14,14,15	0.48	0	17,19,21	1.46	4 (23%)
3	A1IJY	A	801	9	35,35,35	2.90	14 (40%)	43,50,50	2.62	20 (46%)
8	NAG	A	815	1	14,14,15	0.53	0	17,19,21	1.68	8 (47%)
5	EDO	A	809	-	3,3,3	0.25	0	2,2,2	0.24	0
11	1PE	B	810	-	15,15,15	0.45	0	14,14,14	0.53	0
11	1PE	B	802	-	15,15,15	0.56	0	14,14,14	0.68	0
8	NAG	B	811	-	14,14,15	0.51	0	17,19,21	1.30	3 (17%)
5	EDO	B	809	-	3,3,3	0.23	0	2,2,2	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	B	816	1	14,14,15	0.58	0	17,19,21	1.67	4 (23%)
8	NAG	B	812	-	14,14,15	0.48	0	17,19,21	1.03	2 (11%)
3	A1IJY	B	801	9	35,35,35	3.02	14 (40%)	43,50,50	2.44	23 (53%)
4	PEG	A	804	-	6,6,6	0.18	0	5,5,5	0.07	0
4	PEG	B	803	-	6,6,6	0.19	0	5,5,5	0.19	0
5	EDO	A	803	-	3,3,3	0.05	0	2,2,2	0.57	0
8	NAG	B	817	-	14,14,15	0.50	0	17,19,21	1.47	3 (17%)
5	EDO	B	808	-	3,3,3	0.43	0	2,2,2	1.02	0
6	PGE	A	810	-	9,9,9	0.23	0	8,8,8	0.26	0
8	NAG	A	816	-	14,14,15	0.43	0	17,19,21	0.70	0
4	PEG	A	802	-	6,6,6	0.66	0	5,5,5	0.59	0
13	FUC	B	818	-	10,10,11	0.61	0	14,14,16	1.25	2 (14%)
4	PEG	A	805	-	6,6,6	0.26	0	5,5,5	0.37	0
6	PGE	A	806	-	9,9,9	0.29	0	8,8,8	0.26	0
4	PEG	B	807	-	6,6,6	0.29	0	5,5,5	0.13	0
6	PGE	B	806	-	9,9,9	0.32	0	8,8,8	0.26	0
7	P6G	A	808	-	18,18,18	0.42	0	17,17,17	0.55	0
12	PG4	B	804	-	12,12,12	0.26	0	11,11,11	0.37	0
8	NAG	A	814	1	14,14,15	0.50	0	17,19,21	3.91	6 (35%)
5	EDO	B	805	-	3,3,3	0.94	0	2,2,2	1.18	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
6	PGE	A	807	-	-	3/7/7/7	-
8	NAG	A	811	-	-	2/6/23/26	0/1/1/1
8	NAG	B	815	1	-	2/6/23/26	0/1/1/1
3	A1IJY	A	801	9	-	6/36/56/56	0/3/3/3
8	NAG	A	815	1	-	2/6/23/26	0/1/1/1
5	EDO	A	809	-	-	1/1/1/1	-
11	1PE	B	810	-	-	6/13/13/13	-
11	1PE	B	802	-	-	7/13/13/13	-
8	NAG	B	811	-	-	0/6/23/26	0/1/1/1
5	EDO	B	809	-	-	1/1/1/1	-
8	NAG	B	816	1	-	0/6/23/26	0/1/1/1
8	NAG	B	812	-	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1IJY	B	801	9	-	8/36/56/56	0/3/3/3
4	PEG	A	804	-	-	1/4/4/4	-
4	PEG	B	803	-	-	4/4/4/4	-
5	EDO	A	803	-	-	0/1/1/1	-
8	NAG	B	817	-	-	1/6/23/26	0/1/1/1
5	EDO	B	808	-	-	0/1/1/1	-
6	PGE	A	810	-	-	4/7/7/7	-
8	NAG	A	816	-	-	2/6/23/26	0/1/1/1
4	PEG	A	802	-	-	3/4/4/4	-
13	FUC	B	818	-	-	-	0/1/1/1
4	PEG	A	805	-	-	2/4/4/4	-
6	PGE	A	806	-	-	5/7/7/7	-
4	PEG	B	807	-	-	3/4/4/4	-
6	PGE	B	806	-	-	4/7/7/7	-
7	P6G	A	808	-	-	9/16/16/16	-
12	PG4	B	804	-	-	7/10/10/10	-
8	NAG	A	814	1	-	2/6/23/26	0/1/1/1
5	EDO	B	805	-	-	1/1/1/1	-

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	A1IJY	C06-N10	-9.04	1.35	1.47
3	A	801	A1IJY	C06-N10	-8.19	1.36	1.47
3	A	801	A1IJY	C09-N10	6.95	1.61	1.47
3	A	801	A1IJY	C27-N26	6.71	1.60	1.47
3	B	801	A1IJY	C09-N10	5.99	1.59	1.47

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	814	NAG	C2-N2-C7	-13.59	103.55	122.90
3	A	801	A1IJY	O23-C22-O24	-6.30	109.79	124.09
3	A	801	A1IJY	C19-C20-C12	-5.82	114.01	120.78
3	B	801	A1IJY	C14-C13-C12	-5.70	114.15	120.78
3	A	801	A1IJY	C13-C14-C15	-5.45	114.43	120.78

There are no chirality outliers.

5 of 88 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	A1IJY	N04-C05-C06-C07
3	B	801	A1IJY	N04-C05-C06-C07
3	B	801	A1IJY	C22-C05-C06-C07
8	A	816	NAG	O7-C7-N2-C2
3	B	801	A1IJY	C14-C15-C16-O18

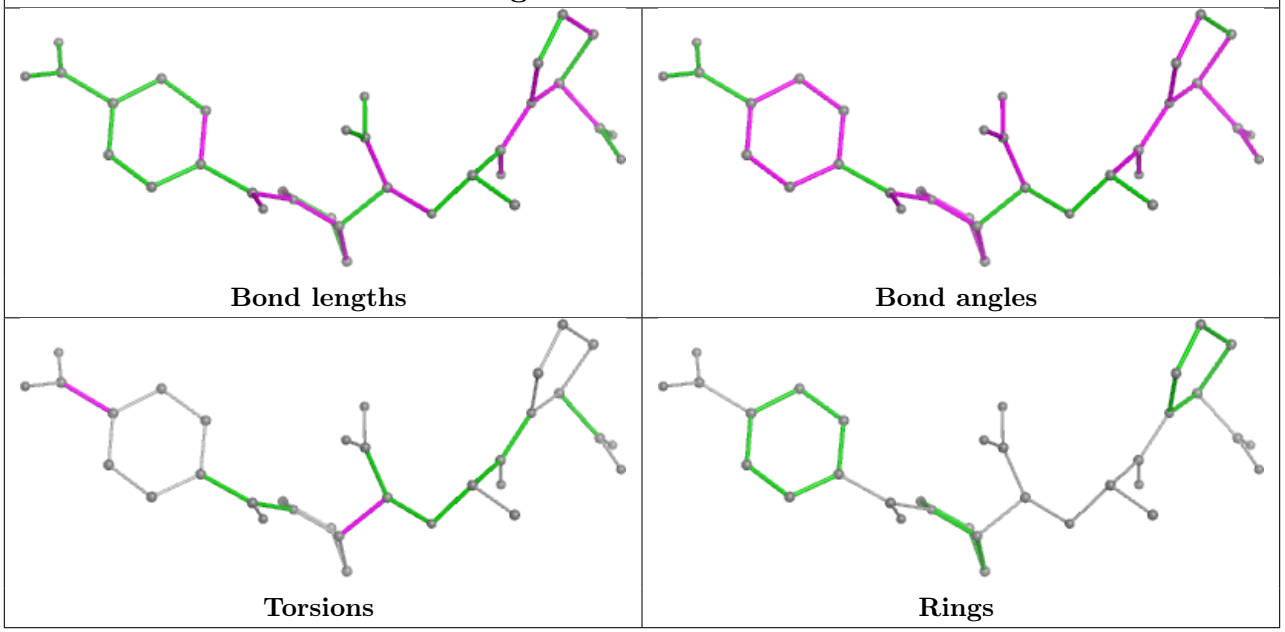
There are no ring outliers.

20 monomers are involved in 50 short contacts:

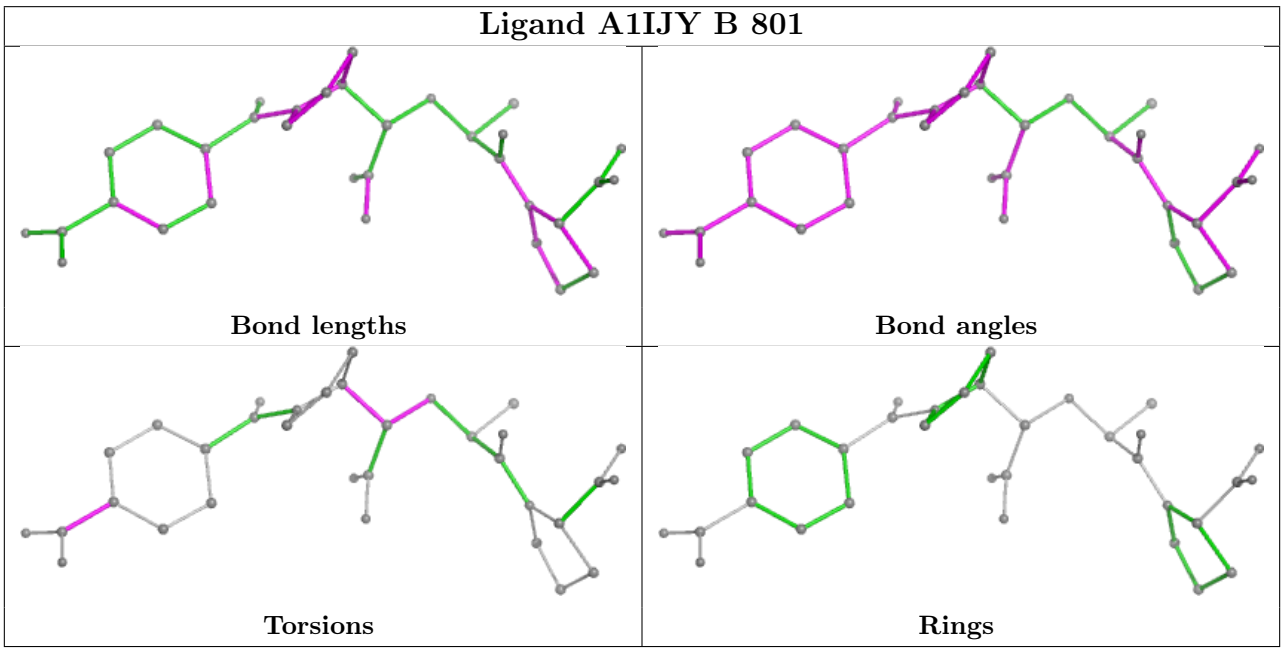
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	807	PGE	4	0
8	A	811	NAG	3	0
8	B	815	NAG	1	0
8	A	815	NAG	4	0
5	A	809	EDO	1	0
11	B	810	1PE	2	0
11	B	802	1PE	3	0
8	B	811	NAG	10	0
5	B	809	EDO	3	0
8	B	816	NAG	4	0
8	B	812	NAG	3	0
4	B	803	PEG	1	0
8	B	817	NAG	2	0
6	A	810	PGE	4	0
8	A	816	NAG	4	0
13	B	818	FUC	2	0
6	B	806	PGE	1	0
7	A	808	P6G	4	0
12	B	804	PG4	4	0
5	B	805	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

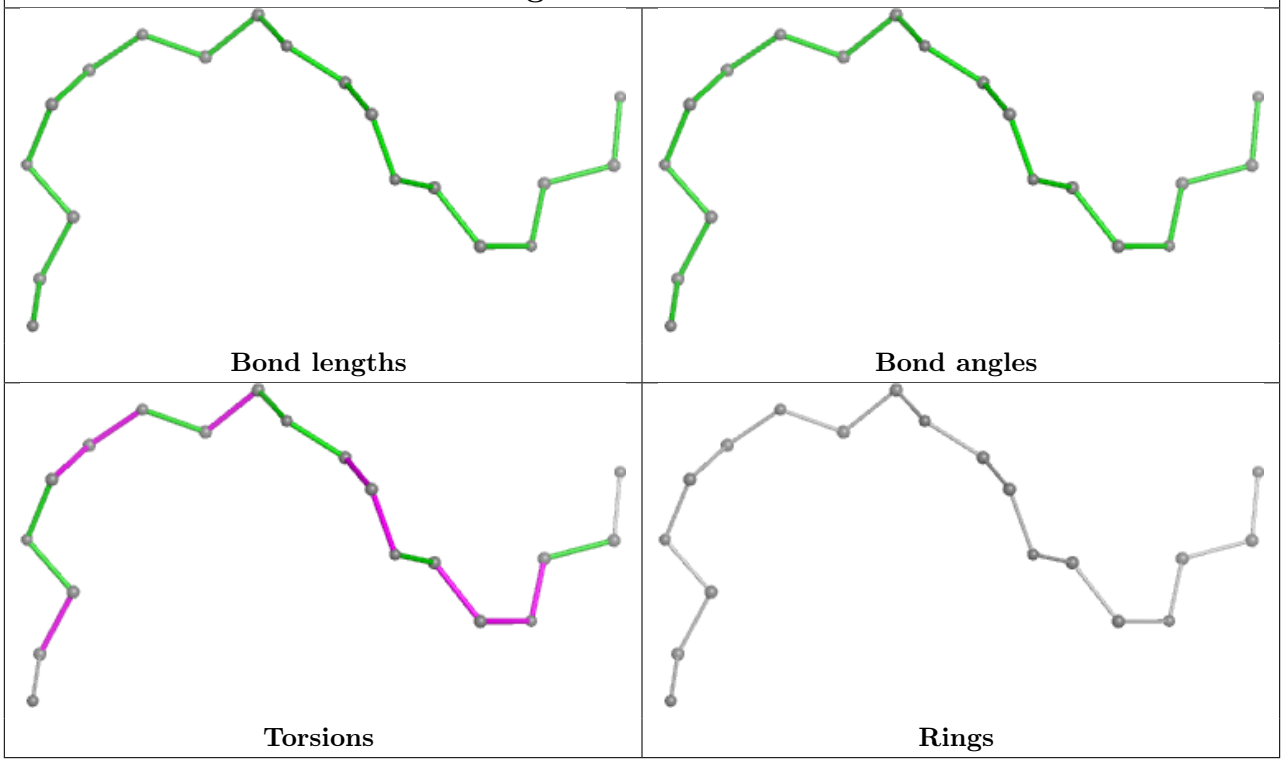
Ligand A1IJY A 801



Ligand A1IJY B 801



Ligand P6G A 808



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	603/628 (96%)	-0.34	3 (0%) 87 88	11, 33, 62, 105	13 (2%)
1	B	603/628 (96%)	-0.42	7 (1%) 76 78	9, 30, 54, 99	6 (0%)
All	All	1206/1256 (96%)	-0.38	10 (0%) 82 84	9, 32, 59, 105	19 (1%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	129	LEU	4.5
1	B	129	LEU	3.8
1	B	608	PRO	3.1
1	B	607	TYR	2.6
1	B	135	THR	2.6

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

SUGAR-RSR INFOmissingINFO

6.4 Ligands

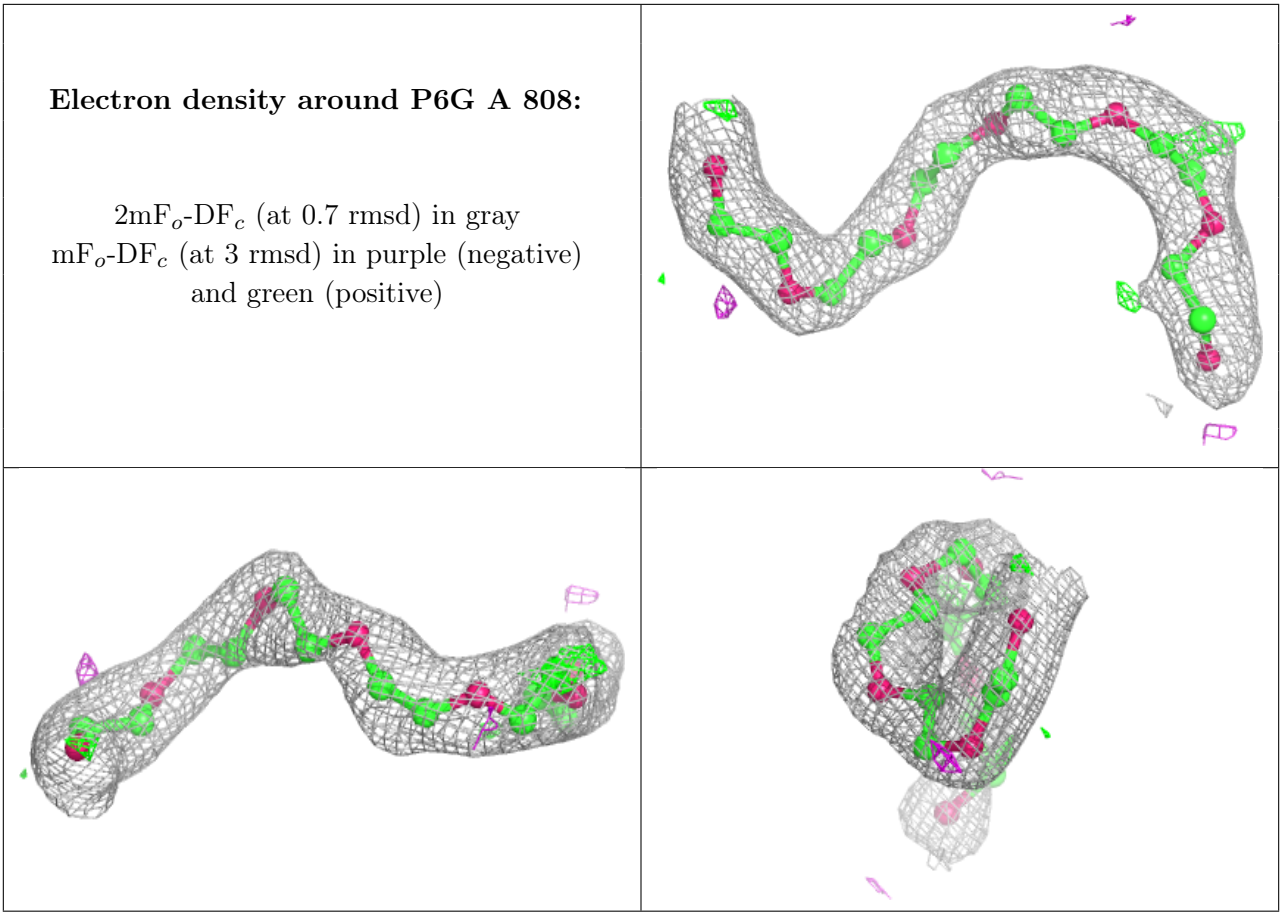
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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
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.

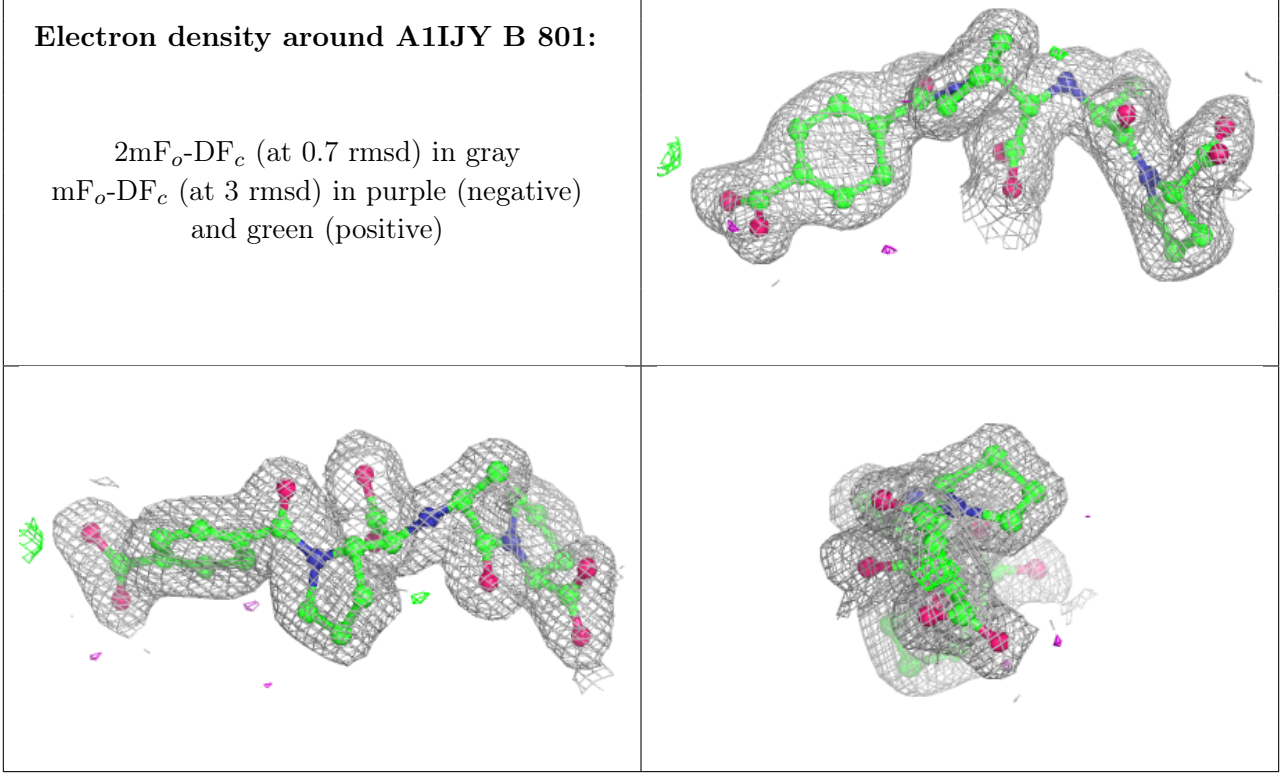
Electron density around P6G A 808:

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



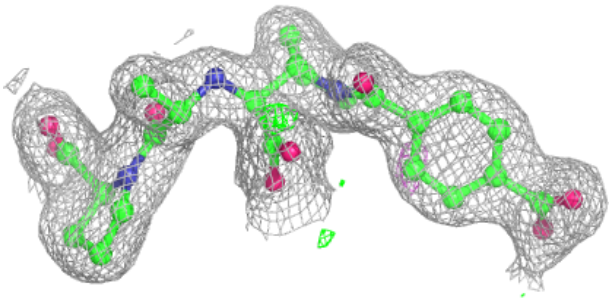
Electron density around A1IJY B 801:

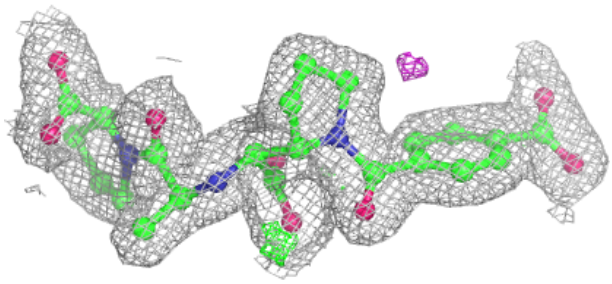
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

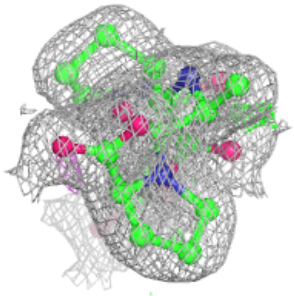


Electron density around A1IJY A 801:

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

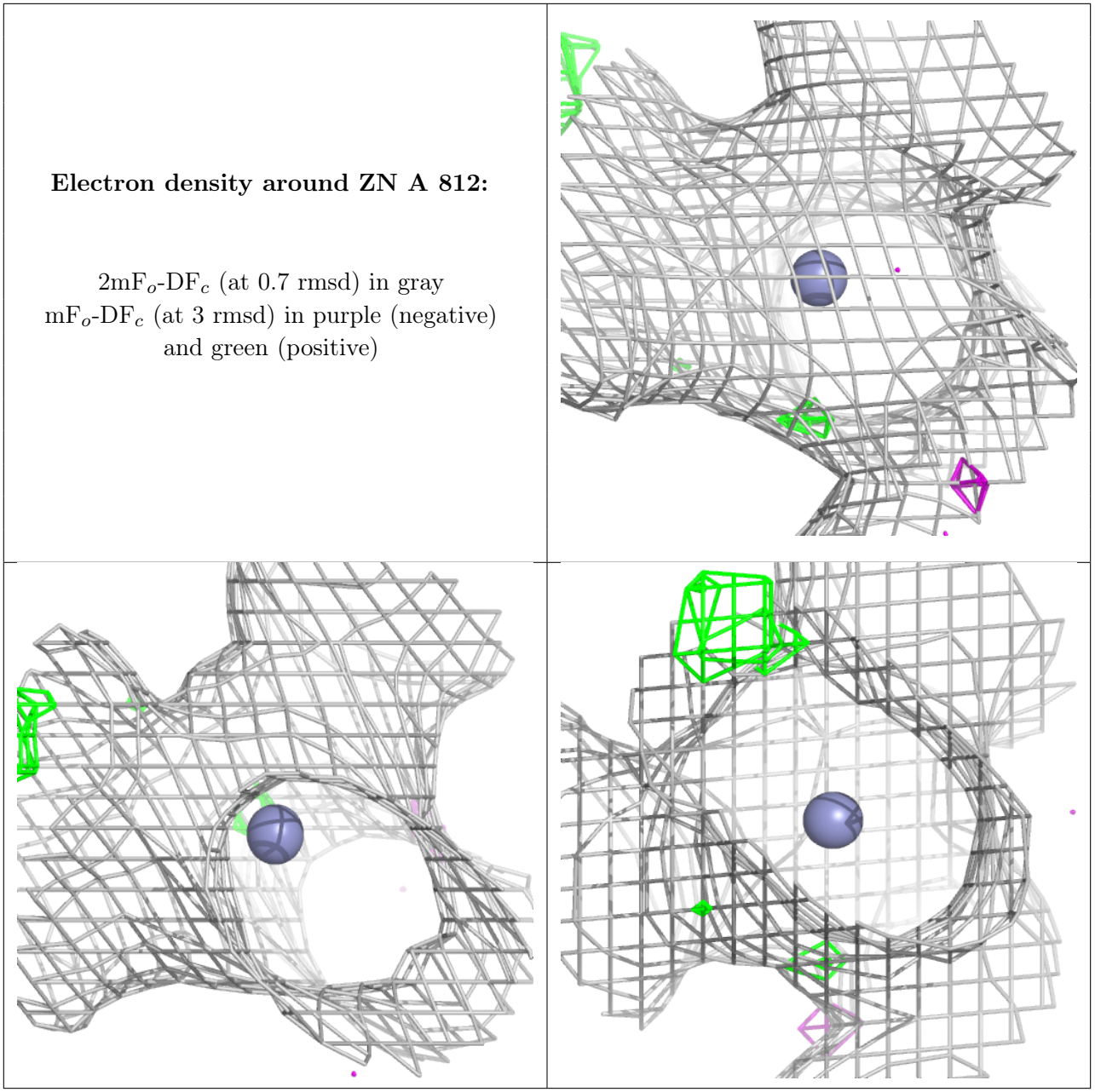






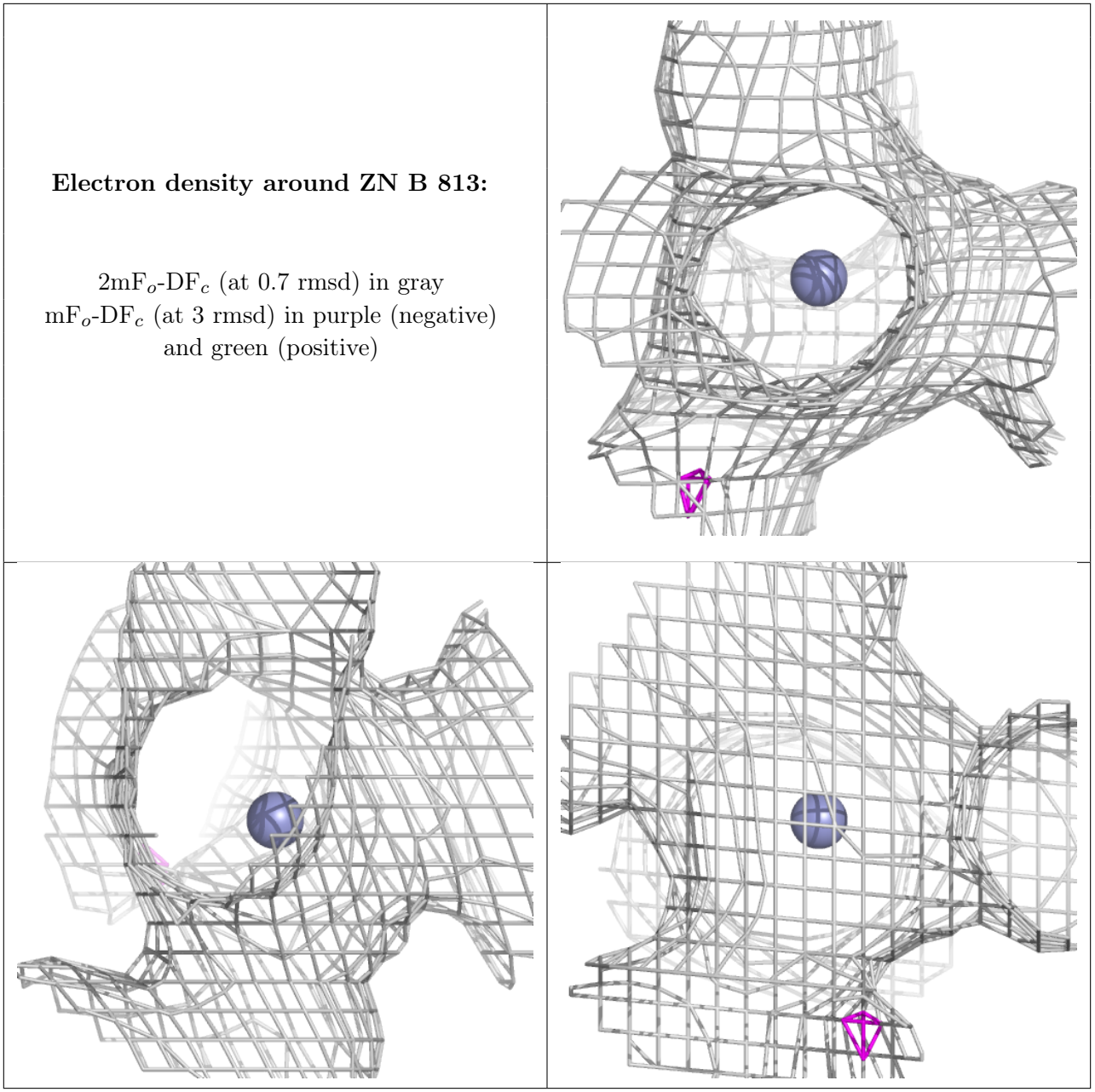
Electron density around ZN A 812:

$2mF_o$-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.