



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 01:16 PM UTC

PDB ID : 6M5E / pdb_00006m5e
Title : Human serum albumin with cyclic peptide dalbavancin
Authors : Ito, S.; Senoo, A.; Nagatoishi, S.; Ohue, M.; Yamamoto, M.; Tsumoto, K.;
Wakui, N.
Deposited on : 2020-03-10
Resolution : 2.80 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 ⓘ 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

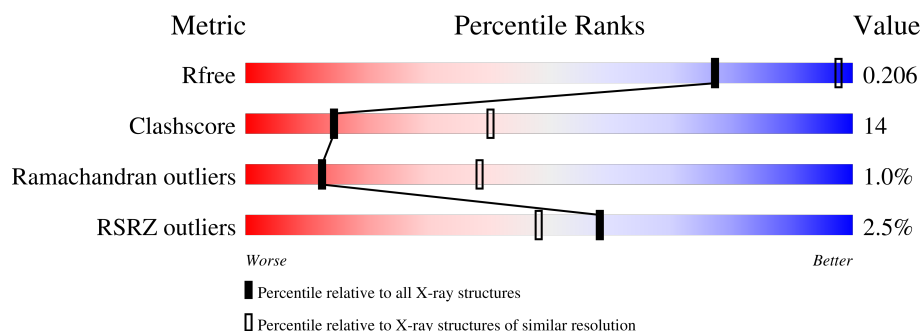
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	585	% 79% 20% .
1	B	585	5% 73% 26% ..
1	C	585	% 79% 20% .
2	F	8	25% 25% 50%
2	G	8	25% 38% 38%
2	H	8	25% 38% 38%

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Mol	Chain	Length	Quality of chain
3	I	8	
3	J	8	

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
2	5PG	F	1	X	-	-	-
2	D4P	F	4	X	-	-	-
2	OMZ	F	6	X	-	-	-
2	D3P	F	7	X	-	-	-
2	5PG	G	1	X	-	-	-
2	D4P	G	4	X	-	-	-
2	OMZ	G	6	X	-	-	-
2	D3P	G	7	X	-	-	-
2	5PG	H	1	X	-	-	-
2	D4P	H	4	X	-	-	-
2	OMZ	H	6	X	-	-	-
2	D3P	H	7	X	-	-	-
5	F8F	F	101	X	-	-	-
5	F8F	G	101	X	-	-	-
5	F8F	H	101	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14585 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 Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	0	0
			4618	2914	781	882	41			
1	B	581	Total	C	N	O	S	0	0	0
			4604	2905	778	880	41			
1	C	581	Total	C	N	O	S	0	0	0
			4618	2915	781	881	41			

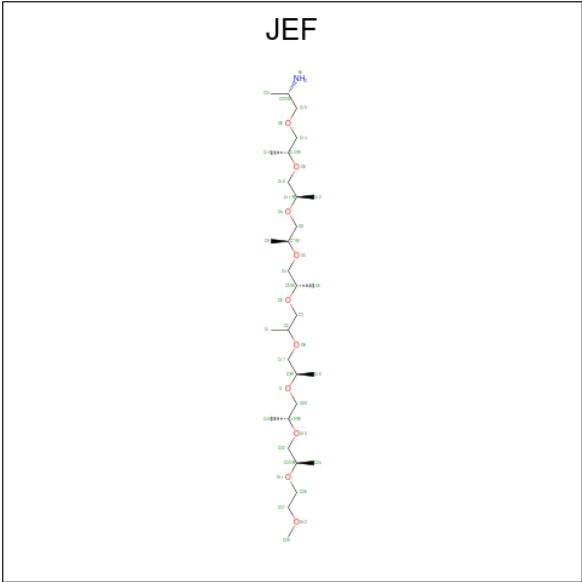
- Molecule 2 is a protein called dalbavancin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	8	Total	C	Cl	N	O	0	0	0
			92	64	2	9	17			
2	G	8	Total	C	Cl	N	O	0	0	0
			92	64	2	9	17			
2	H	8	Total	C	Cl	N	O	0	0	0
			92	64	2	9	17			

- Molecule 3 is a protein called dalbavancin.

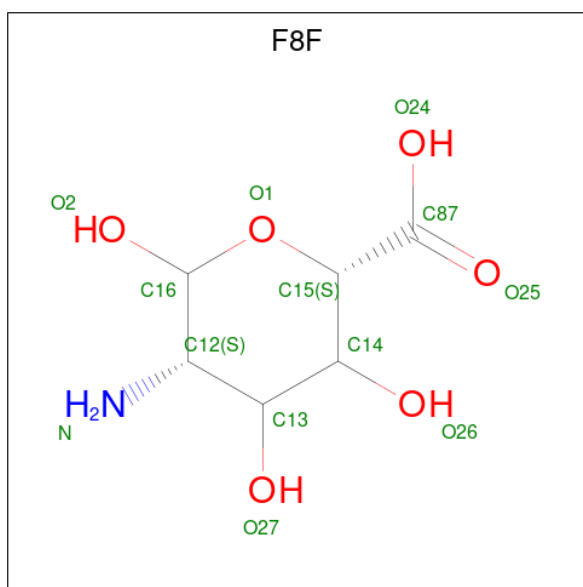
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	8	Total	C	Cl	N	O	0	0	0
			92	64	2	9	17			
3	J	8	Total	C	Cl	N	O	0	0	0
			92	64	2	9	17			

- Molecule 4 is O-(O-(2-AMINOPROPYL)-O'-(2-METHOXYETHYL)POLYPROPYLENE GLYCOL 500) (CCD ID: JEF) (formula: C₃₀H₆₃NO₁₀).



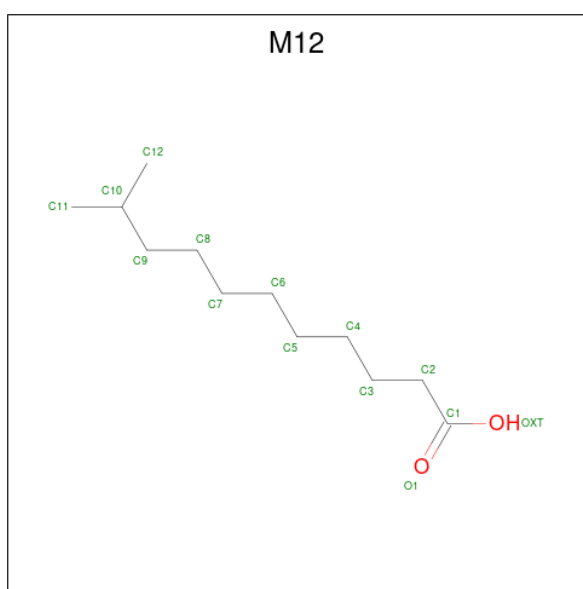
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			17	12	5		
4	A	1	Total	C	O	0	0
			17	12	5		
4	B	1	Total	C	O	0	0
			17	12	5		
4	B	1	Total	C	O	0	0
			17	12	5		
4	C	1	Total	C	O	0	0
			17	12	5		
4	C	1	Total	C	O	0	0
			17	12	5		

- Molecule 5 is (2S,5S)-5-azanyl-3,4,6-tris(oxidanyl)oxane-2-carboxylic acid (CCD ID: F8F) (formula: C₆H₁₁NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	F	1	Total	C	N	O	0	0
			12	6	1	5		
5	G	1	Total	C	N	O	0	0
			12	6	1	5		
5	H	1	Total	C	N	O	0	0
			12	6	1	5		

- Molecule 6 is 10-METHYLUNDECANOIC ACID (CCD ID: M12) (formula: $C_{12}H_{24}O_2$).



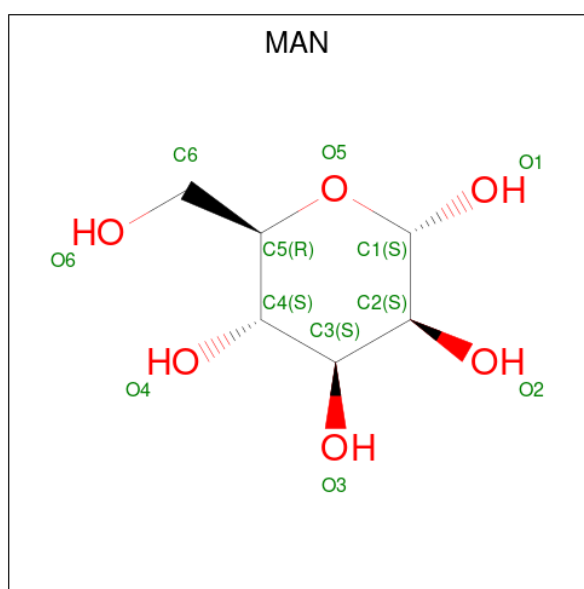
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	C	O	0	0
			13	12	1		

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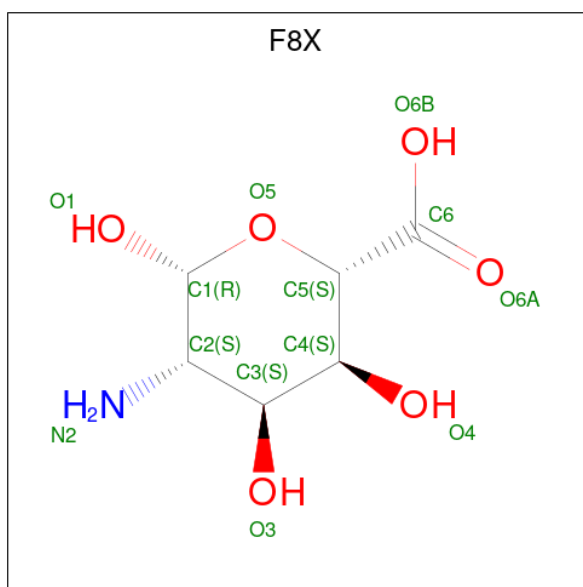
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	C	O	0	0
			13	12	1		
6	H	1	Total	C	O	0	0
			13	12	1		
6	I	1	Total	C	O	0	0
			13	12	1		
6	J	1	Total	C	O	0	0
			13	12	1		

- Molecule 7 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$).



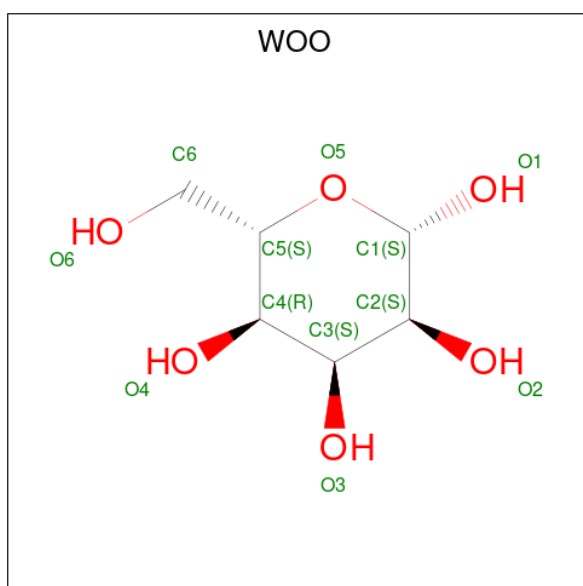
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total	C	O	0	0
			11	6	5		
7	G	1	Total	C	O	0	0
			11	6	5		
7	H	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is 2-amino-2-deoxy-beta-D-altropyranuronic acid (CCD ID: F8X) (formula: $C_6H_{11}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	I	1	Total	C	N	O	0	0
			12	6	1	5		
8	J	1	Total	C	N	O	0	0
			12	6	1	5		

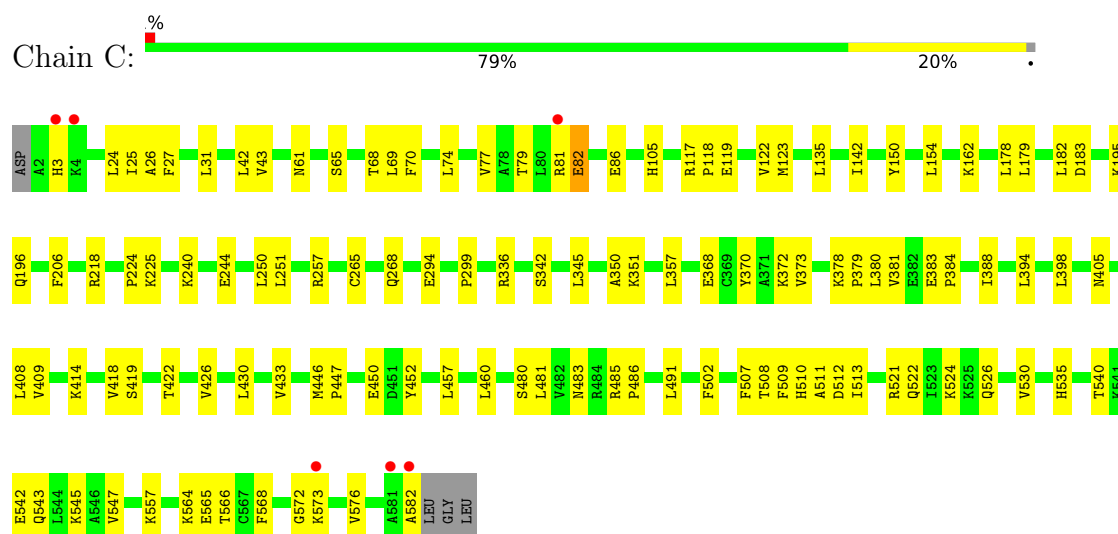
- Molecule 9 is beta-L-allopyranose (CCD ID: WOO) (formula: $C_6H_{12}O_6$).



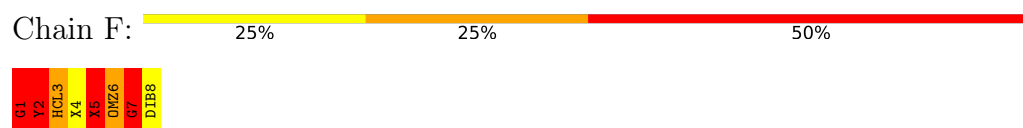
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	I	1	Total	C	O	0	0
			11	6	5		
9	J	1	Total	C	O	0	0
			11	6	5		

- Molecule 10 is water.

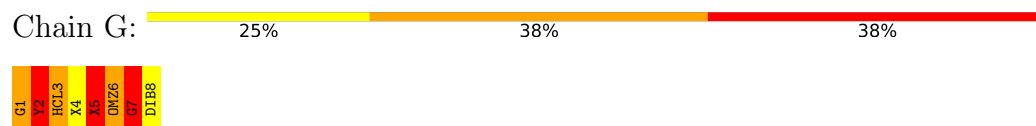
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	F	1	Total 1	O 1	0	0
10	G	1	Total 1	O 1	0	0
10	H	1	Total 1	O 1	0	0



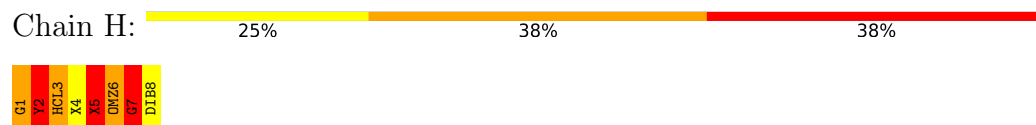
- Molecule 2: dalbavancin



- Molecule 2: dalbavancin



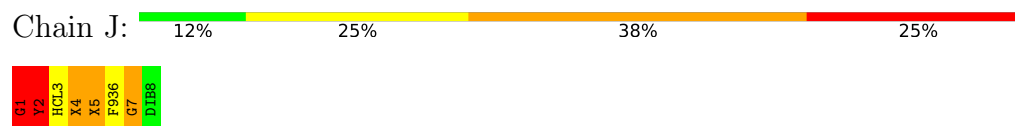
- Molecule 2: dalbavancin



- Molecule 3: dalbavancin



- Molecule 3: dalbavancin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	197.05Å 125.68Å 125.74Å 90.00° 90.32° 90.00°	Depositor
Resolution (Å)	45.78 – 2.80 45.78 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.78-2.80) 94.9 (45.78-2.80)	Depositor EDS
R_{merge}	0.47	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.17	Depositor
R, R_{free}	0.180 , 0.228 (Not available) , 0.206	Depositor DCC
R_{free} test set	3777 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14585	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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: D3P, HCL, OMZ, M12, 5PG, DIB, F8F, WOO, JEF, F8X, F93, MAN, D4P

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	0.45	0/4707	0.70	3/6350 (0.0%)
1	B	0.43	0/4694	0.71	6/6337 (0.1%)
1	C	0.48	0/4708	0.72	0/6351
2	F	0.37	0/12	1.22	0/15
2	G	0.32	0/12	1.30	0/15
2	H	0.29	0/12	1.08	0/15
3	I	0.35	0/12	0.76	0/15
3	J	0.32	0/12	0.79	0/15
All	All	0.45	0/14169	0.71	9/19113 (0.0%)

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
2	F	4	6
2	G	4	6
2	H	4	6
3	I	0	5
3	J	0	5
All	All	12	28

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	559	CYS	N-CA-C	8.82	116.01	108.78
1	A	53	CYS	CA-CB-SG	-8.18	95.58	114.40
1	A	62	CYS	CA-CB-SG	-8.07	95.84	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	559	CYS	CB-CA-C	-6.61	107.56	117.07
1	B	559	CYS	CA-C-O	6.51	121.72	117.94

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	1	5PG	CA
2	F	4	D4P	CA
2	F	6	OMZ	CB
2	F	7	D3P	CA
2	G	1	5PG	CA

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	1	5PG	Peptide
2	F	2	TYR	Peptide,Sidechain
2	F	5	D4P	Mainchain,Peptide
2	F	7	D3P	Peptide
2	G	1	5PG	Peptide

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	4618	0	4529	101	0
1	B	4604	0	4499	132	0
1	C	4618	0	4534	121	0
2	F	92	0	47	7	0
2	G	92	0	45	7	0
2	H	92	0	44	6	0
3	I	92	0	43	10	0
3	J	92	0	42	12	0
4	A	34	0	50	13	0
4	B	34	0	50	12	0
4	C	34	0	50	15	0
5	F	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	12	0	0	0	0
5	H	12	0	0	0	0
6	F	13	0	23	2	0
6	G	13	0	23	2	0
6	H	13	0	23	2	0
6	I	13	0	23	1	0
6	J	13	0	23	0	0
7	F	11	0	10	1	0
7	G	11	0	10	1	0
7	H	11	0	10	1	0
8	I	12	0	0	1	0
8	J	12	0	0	0	0
9	I	11	0	10	2	0
9	J	11	0	10	2	0
10	F	1	0	0	0	0
10	G	1	0	0	0	0
10	H	1	0	0	0	0
All	All	14585	0	14098	400	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 14.

The worst 5 of 400 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:C:540:THR:HG22	1:C:543:GLN:H	1.15	1.09
1:B:539:ALA:HB1	1:B:544:LEU:HD21	1.26	1.07
1:C:150:TYR:HB2	1:C:196:GLN:HG3	1.42	1.00
1:B:518:GLU:HA	1:B:521:ARG:HD2	1.46	0.98
1:C:394:LEU:HD22	1:C:398:LEU:HD22	1.56	0.88

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	579/585 (99%)	559 (96%)	20 (4%)	0	100	100
1	B	579/585 (99%)	547 (94%)	23 (4%)	9 (2%)	7	27
1	C	579/585 (99%)	560 (97%)	15 (3%)	4 (1%)	18	47
2	F	1/8 (12%)	0	0	1 (100%)	0	0
2	G	1/8 (12%)	0	0	1 (100%)	0	0
2	H	1/8 (12%)	0	0	1 (100%)	0	0
3	I	1/8 (12%)	0	0	1 (100%)	0	0
3	J	1/8 (12%)	0	0	1 (100%)	0	0
All	All	1742/1795 (97%)	1666 (96%)	58 (3%)	18 (1%)	12	38

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	539	ALA
1	B	541	LYS
1	B	563	ASP
1	B	566	THR
1	C	3	HIS

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

30 non-standard protein/DNA/RNA residues 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	D4P	F	5	2	10,11,12	1.70	1 (10%)	11,14,16	0.80	0
3	F93	J	6	3	12,14,15	0.54	0	17,19,21	0.76	0
2	D3P	H	7	2	11,12,13	0.93	1 (9%)	11,16,18	1.18	1 (9%)
2	5PG	G	1	2	11,12,13	0.64	0	10,15,17	0.72	0
3	HCL	J	3	3	11,13,14	1.01	1 (9%)	13,18,20	0.46	0
2	D3P	G	7	2	11,12,13	0.94	1 (9%)	11,16,18	1.24	1 (9%)
3	D3P	I	7	3	11,12,13	0.81	0	11,16,18	1.77	2 (18%)
2	D4P	F	4	2,5	10,11,12	0.89	1 (10%)	11,14,16	0.68	0
2	D3P	F	7	2	11,12,13	0.85	0	11,16,18	1.06	1 (9%)
2	HCL	G	3	2	11,13,14	1.46	1 (9%)	13,18,20	0.88	1 (7%)
2	D4P	H	4	2,5	10,11,12	0.83	1 (10%)	11,14,16	0.73	0
3	D4P	J	5	3	10,11,12	0.73	0	11,14,16	0.91	0
2	D4P	G	5	2	10,11,12	1.22	1 (10%)	11,14,16	0.78	0
3	D4P	I	5	3	10,11,12	0.79	0	11,14,16	0.81	0
2	OMZ	G	6	2	12,14,15	0.51	0	17,19,21	2.30	3 (17%)
2	5PG	F	1	2	11,12,13	1.13	1 (9%)	10,15,17	0.74	0
2	5PG	H	1	2	11,12,13	0.67	0	10,15,17	0.76	0
3	F93	I	6	3	12,14,15	0.61	0	17,19,21	0.69	0
3	5PG	J	1	3	11,12,13	1.03	1 (9%)	10,15,17	0.42	0
3	D3P	J	7	3	11,12,13	0.86	0	11,16,18	1.63	2 (18%)
2	OMZ	F	6	2	12,14,15	0.56	0	17,19,21	2.34	3 (17%)
3	5PG	I	1	3	11,12,13	0.91	1 (9%)	10,15,17	0.41	0
2	HCL	H	3	2	11,13,14	1.14	1 (9%)	13,18,20	0.90	1 (7%)
3	HCL	I	3	3	11,13,14	0.89	1 (9%)	13,18,20	0.37	0
3	D4P	J	4	3	10,11,12	1.31	1 (10%)	11,14,16	0.72	0
2	OMZ	H	6	2	12,14,15	0.45	0	17,19,21	2.32	3 (17%)
2	D4P	G	4	2,5	10,11,12	1.35	1 (10%)	11,14,16	0.90	1 (9%)
2	D4P	H	5	2	10,11,12	0.94	1 (10%)	11,14,16	0.75	0
3	D4P	I	4	3	10,11,12	0.82	1 (10%)	11,14,16	0.89	0
2	HCL	F	3	2	11,13,14	1.53	1 (9%)	13,18,20	1.00	2 (15%)

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	D4P	F	5	2	-	0/4/6/8	0/1/1/1
3	F93	J	6	3	-	5/9/10/12	0/1/1/1
2	D3P	H	7	2	1/1/1/2	0/4/6/8	0/1/1/1
2	5PG	G	1	2	1/1/1/3	1/5/8/10	0/1/1/1
3	HCL	J	3	3	-	4/4/6/8	0/1/1/1
2	D3P	G	7	2	1/1/1/2	0/4/6/8	0/1/1/1
3	D3P	I	7	3	-	0/4/6/8	0/1/1/1
2	D4P	F	4	2,5	1/1/1/2	1/4/6/8	0/1/1/1
2	D3P	F	7	2	1/1/1/2	0/4/6/8	0/1/1/1
2	HCL	G	3	2	-	0/4/6/8	0/1/1/1
2	D4P	H	4	2,5	1/1/1/2	1/4/6/8	0/1/1/1
3	D4P	J	5	3	-	0/4/6/8	0/1/1/1
2	D4P	G	5	2	-	0/4/6/8	0/1/1/1
3	D4P	I	5	3	-	0/4/6/8	0/1/1/1
2	OMZ	G	6	2	1/1/2/3	3/9/10/12	0/1/1/1
2	5PG	F	1	2	1/1/1/3	1/5/8/10	0/1/1/1
2	5PG	H	1	2	1/1/1/3	1/5/8/10	0/1/1/1
3	F93	I	6	3	-	5/9/10/12	0/1/1/1
3	5PG	J	1	3	-	0/5/8/10	0/1/1/1
3	D3P	J	7	3	-	0/4/6/8	0/1/1/1
2	OMZ	F	6	2	1/1/2/3	3/9/10/12	0/1/1/1
3	5PG	I	1	3	-	0/5/8/10	0/1/1/1
2	HCL	H	3	2	-	1/4/6/8	0/1/1/1
3	HCL	I	3	3	-	4/4/6/8	0/1/1/1
3	D4P	J	4	3	-	0/4/6/8	0/1/1/1
2	OMZ	H	6	2	1/1/2/3	4/9/10/12	0/1/1/1
2	D4P	G	4	2,5	1/1/1/2	1/4/6/8	0/1/1/1
2	D4P	H	5	2	-	0/4/6/8	0/1/1/1
3	D4P	I	4	3	-	0/4/6/8	0/1/1/1
2	HCL	F	3	2	-	0/4/6/8	0/1/1/1

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	5	D4P	CA-C	4.95	1.59	1.51
2	F	3	HCL	CA-C	4.76	1.59	1.51
2	G	3	HCL	CA-C	4.38	1.58	1.51
3	J	4	D4P	CA-C	-3.95	1.44	1.51
2	G	4	D4P	CA-C	3.94	1.57	1.51

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	6	OMZ	OC-CB-CA	7.45	123.85	107.49
2	F	6	OMZ	OC-CB-CA	7.30	123.53	107.49
2	G	6	OMZ	OC-CB-CA	6.95	122.76	107.49
3	I	7	D3P	C1-CA-C	-4.38	99.79	112.09
2	G	6	OMZ	OC-CB-CG	4.27	120.47	111.20

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	1	5PG	CA
2	G	1	5PG	CA
2	H	1	5PG	CA
2	F	4	D4P	CA
2	G	4	D4P	CA

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1	5PG	CB-CA-N-CN
2	G	1	5PG	CB-CA-N-CN
2	H	1	5PG	CB-CA-N-CN
2	H	3	HCL	C2-C1-CA-C
2	F	6	OMZ	N-CA-CB-CG

There are no ring outliers.

24 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	5	D4P	2	0
3	J	6	F93	1	0
2	H	7	D3P	1	0
2	G	1	5PG	4	0
2	G	7	D3P	1	0
3	I	7	D3P	1	0
2	F	7	D3P	1	0
2	G	3	HCL	1	0
3	J	5	D4P	2	0
2	G	5	D4P	1	0
3	I	5	D4P	1	0
2	G	6	OMZ	1	0
2	F	1	5PG	4	0
2	H	1	5PG	4	0
3	J	1	5PG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	7	D3P	5	0
2	F	6	OMZ	2	0
3	I	1	5PG	5	0
2	H	3	HCL	2	0
3	J	4	D4P	2	0
2	H	6	OMZ	1	0
2	H	5	D4P	1	0
3	I	4	D4P	2	0
2	F	3	HCL	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

21 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	M12	G	102	5	11,12,13	0.24	0	11,12,14	0.23	0
7	MAN	F	103	-	11,11,12	0.54	0	15,15,17	3.44	9 (60%)
9	WOO	J	103	-	11,11,12	0.66	0	15,15,17	0.83	0
4	JEF	B	802	-	16,16,40	0.66	0	18,18,48	0.86	0
4	JEF	A	801	-	16,16,40	1.27	1 (6%)	18,18,48	1.02	2 (11%)
4	JEF	B	801	-	16,16,40	1.06	1 (6%)	18,18,48	1.04	1 (5%)
7	MAN	H	103	-	11,11,12	0.50	0	15,15,17	3.35	7 (46%)
6	M12	I	101	8	11,12,13	0.25	0	11,12,14	0.30	0
5	F8F	G	101	6,2	12,12,13	1.45	3 (25%)	12,17,19	4.16	7 (58%)
4	JEF	C	801	-	16,16,40	0.71	0	18,18,48	0.96	0
4	JEF	A	802	-	16,16,40	0.62	1 (6%)	18,18,48	0.98	1 (5%)
8	F8X	I	102	6	12,12,13	0.56	0	12,17,19	1.45	1 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	F8F	F	101	6,2	12,12,13	1.49	3 (25%)	12,17,19	4.15	7 (58%)
6	M12	H	102	5	11,12,13	0.31	0	11,12,14	0.30	0
7	MAN	G	103	-	11,11,12	0.57	0	15,15,17	3.26	7 (46%)
6	M12	J	101	8	11,12,13	0.20	0	11,12,14	0.28	0
8	F8X	J	102	6	12,12,13	1.36	2 (16%)	12,17,19	1.69	2 (16%)
5	F8F	H	101	6,2	12,12,13	1.46	3 (25%)	12,17,19	4.17	7 (58%)
4	JEF	C	802	-	16,16,40	0.96	1 (6%)	18,18,48	0.97	0
9	WOO	I	103	-	11,11,12	0.64	0	15,15,17	0.93	1 (6%)
6	M12	F	102	5	11,12,13	0.27	0	11,12,14	0.21	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	M12	G	102	5	-	4/10/10/11	-
7	MAN	F	103	-	-	1/2/19/22	0/1/1/1
9	WOO	J	103	-	-	0/2/19/22	0/1/1/1
4	JEF	B	802	-	-	5/17/17/46	-
4	JEF	A	801	-	-	7/17/17/46	-
4	JEF	B	801	-	-	5/17/17/46	-
7	MAN	H	103	-	-	1/2/19/22	0/1/1/1
6	M12	I	101	8	-	6/10/10/11	-
5	F8F	G	101	6,2	4/4/5/6	2/4/21/24	0/1/1/1
4	JEF	C	801	-	-	7/17/17/46	-
4	JEF	A	802	-	-	8/17/17/46	-
8	F8X	I	102	6	-	3/4/21/24	0/1/1/1
5	F8F	F	101	6,2	3/3/5/6	2/4/21/24	0/1/1/1
6	M12	H	102	5	-	4/10/10/11	-
7	MAN	G	103	-	-	2/2/19/22	0/1/1/1
6	M12	J	101	8	-	3/10/10/11	-
8	F8X	J	102	6	-	0/4/21/24	0/1/1/1
5	F8F	H	101	6,2	3/3/5/6	2/4/21/24	0/1/1/1
4	JEF	C	802	-	-	7/17/17/46	-
9	WOO	I	103	-	-	2/2/19/22	0/1/1/1
6	M12	F	102	5	-	4/10/10/11	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	JEF	O11-C33	4.47	1.51	1.44
4	B	801	JEF	O-C	3.63	1.49	1.44
5	H	101	F8F	O25-C87	3.56	1.32	1.22
5	G	101	F8F	O25-C87	3.39	1.32	1.22
5	F	101	F8F	O25-C87	3.33	1.32	1.22

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	101	F8F	O26-C14-C15	8.66	129.54	109.76
5	H	101	F8F	O26-C14-C15	8.46	129.09	109.76
5	F	101	F8F	O26-C14-C15	7.88	127.76	109.76
5	F	101	F8F	O27-C13-C12	7.59	124.10	109.90
5	H	101	F8F	O27-C13-C12	7.50	123.92	109.90

5 of 10 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	F	101	F8F	C13
5	F	101	F8F	C14
5	F	101	F8F	C16
5	G	101	F8F	C13
5	G	101	F8F	C14

5 of 75 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	JEF	C34-C33-O11-C36
4	A	801	JEF	O10-C32-C33-O11
4	A	801	JEF	O10-C32-C33-C34
4	A	801	JEF	O10-C19-C20-O
4	A	801	JEF	C40-C19-C20-O

There are no ring outliers.

16 monomers are involved in 55 short contacts:

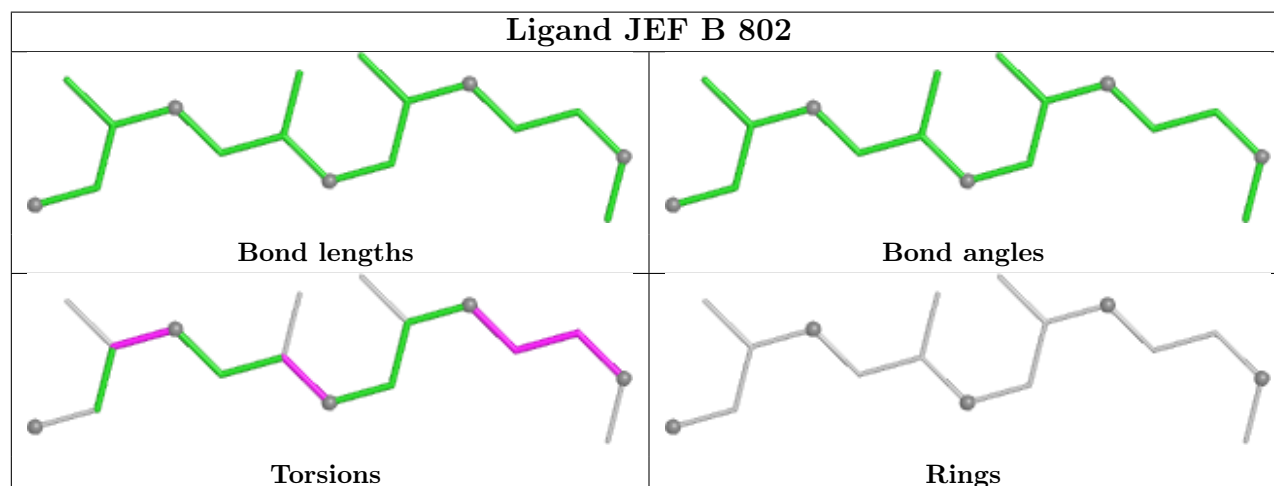
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	102	M12	2	0
7	F	103	MAN	1	0
9	J	103	WOO	2	0
4	B	802	JEF	9	0

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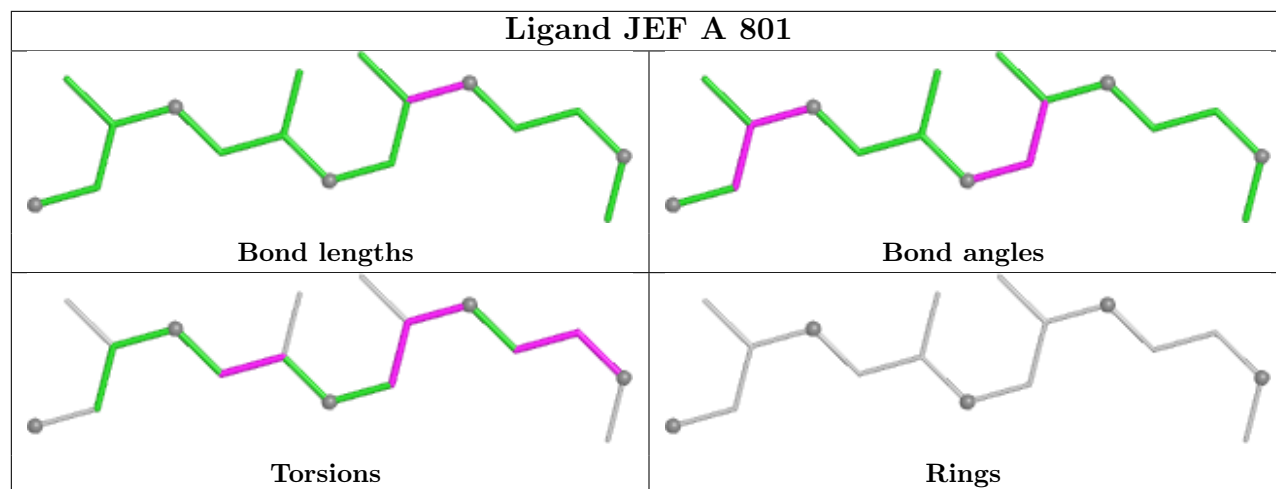
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	JEF	10	0
4	B	801	JEF	3	0
7	H	103	MAN	1	0
6	I	101	M12	1	0
4	C	801	JEF	10	0
4	A	802	JEF	3	0
8	I	102	F8X	1	0
6	H	102	M12	2	0
7	G	103	MAN	1	0
4	C	802	JEF	5	0
9	I	103	WOO	2	0
6	F	102	M12	2	0

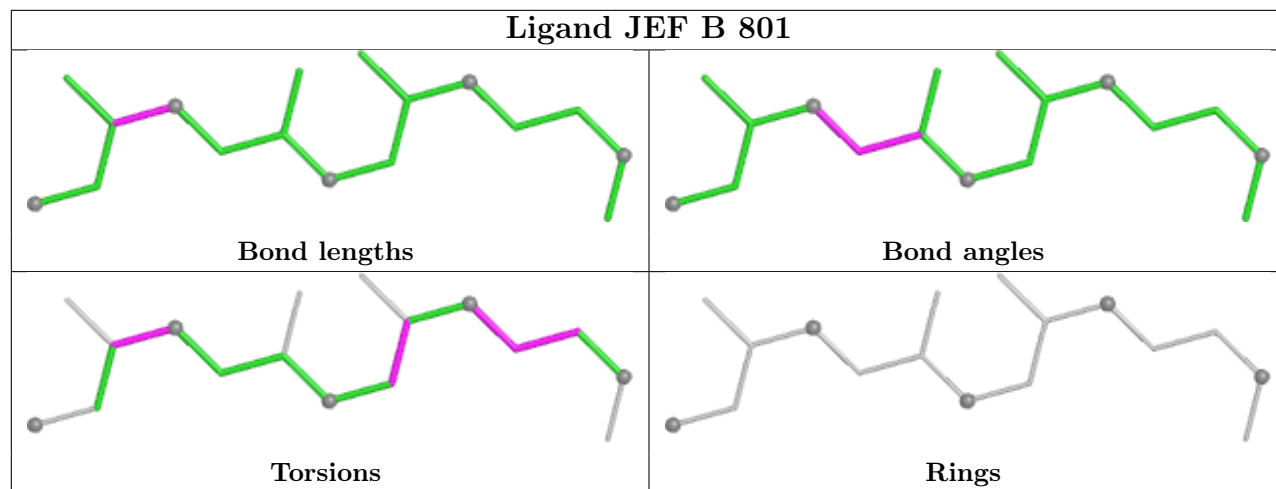
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



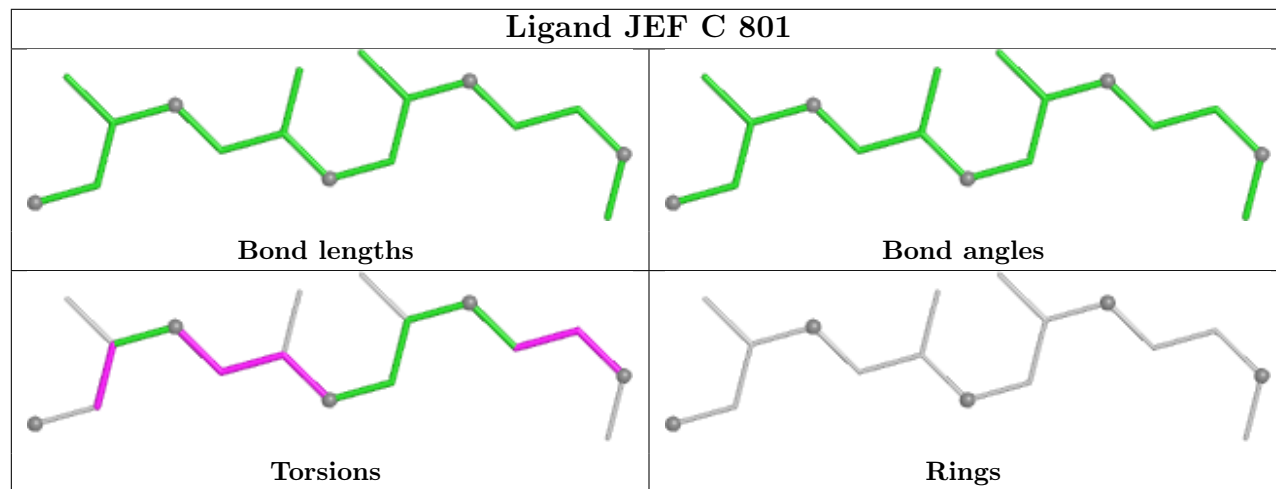
Ligand JEF A 801

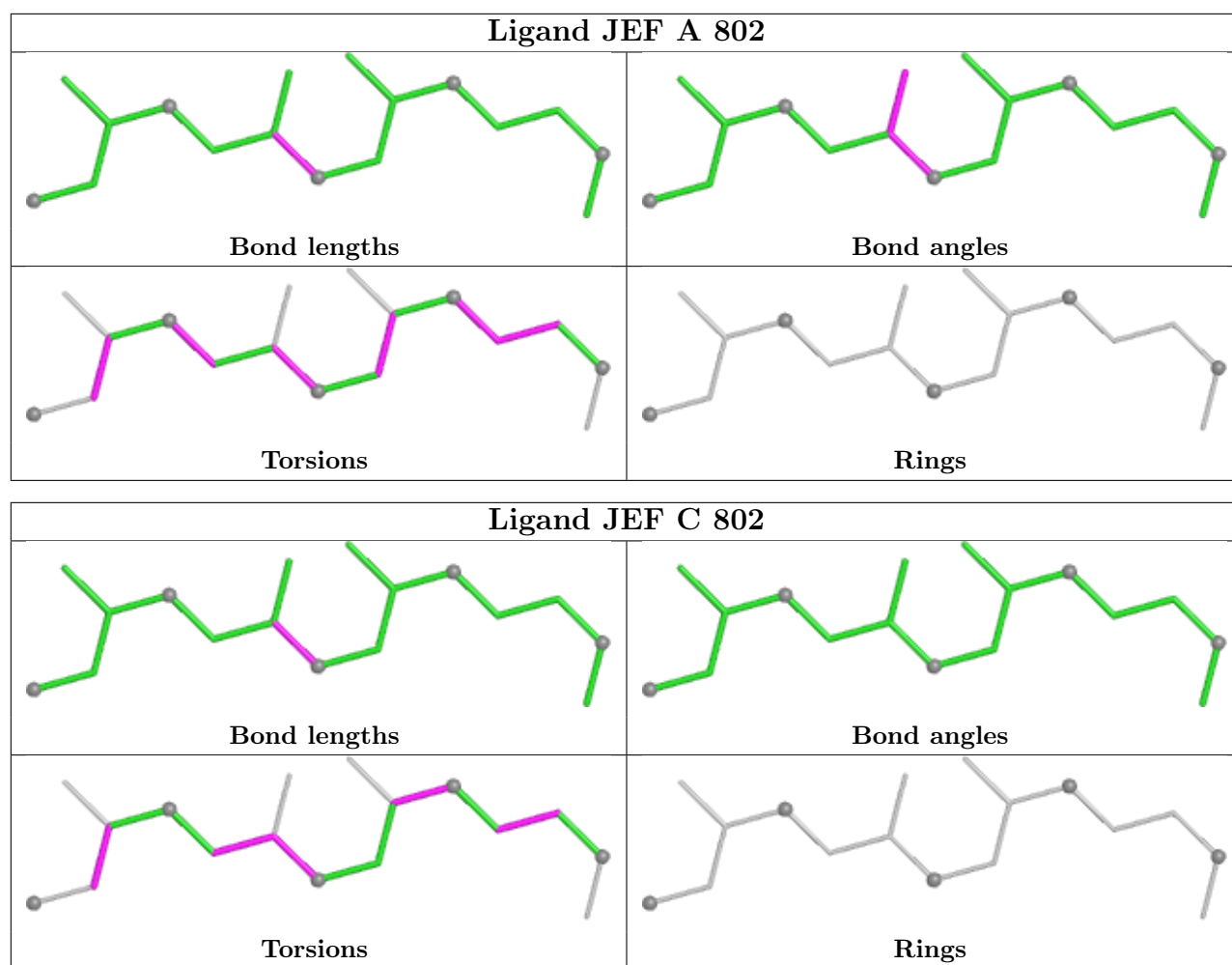


Ligand JEF B 801



Ligand JEF C 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	581/585 (99%)	-0.51	6 (1%) 79 72	32, 54, 99, 190	0
1	B	581/585 (99%)	-0.22	32 (5%) 30 23	29, 59, 174, 221	0
1	C	581/585 (99%)	-0.60	6 (1%) 79 72	29, 50, 95, 141	0
2	F	1/8 (12%)	0.17	0 100 100	92, 92, 92, 92	0
2	G	1/8 (12%)	1.29	0 100 100	101, 101, 101, 101	0
2	H	1/8 (12%)	0.30	0 100 100	83, 83, 83, 83	0
3	I	1/8 (12%)	0.83	0 100 100	73, 73, 73, 73	0
3	J	1/8 (12%)	0.78	0 100 100	64, 64, 64, 64	0
All	All	1748/1795 (97%)	-0.44	44 (2%) 58 48	29, 54, 123, 221	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	LYS	4.0
1	B	575	LEU	4.0
1	C	4	LYS	3.9
1	B	560	LYS	3.6
1	C	81	ARG	3.4

6.2 Non-standard residues in protein, DNA, RNA chains [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	5PG	G	1	12/13	0.64	0.20	102,110,115,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HCL	F	3	13/14	0.64	0.13	92,106,127,143	0
2	HCL	G	3	13/14	0.70	0.11	98,107,118,124	0
2	HCL	H	3	13/14	0.71	0.14	83,98,125,143	0
3	5PG	I	1	12/13	0.73	0.19	83,96,115,120	0
3	5PG	J	1	12/13	0.73	0.20	67,87,107,127	0
2	OMZ	G	6	14/15	0.79	0.14	91,100,107,116	0
2	D4P	G	4	11/12	0.79	0.12	93,103,109,113	0
2	D4P	G	5	11/12	0.79	0.14	71,91,99,100	0
2	5PG	F	1	12/13	0.81	0.12	84,99,110,122	0
3	HCL	I	3	13/14	0.82	0.16	81,88,110,136	0
3	HCL	J	3	13/14	0.83	0.18	78,91,120,139	0
2	5PG	H	1	12/13	0.84	0.13	70,86,91,104	0
2	D3P	G	7	12/13	0.85	0.12	60,82,103,123	0
2	D3P	F	7	12/13	0.87	0.10	69,86,100,102	0
2	D4P	H	5	11/12	0.88	0.10	67,80,88,99	0
2	OMZ	F	6	14/15	0.88	0.14	79,83,96,128	0
2	D4P	H	4	11/12	0.88	0.11	69,74,81,89	0
3	D3P	I	7	12/13	0.90	0.10	62,67,71,82	0
2	D4P	F	5	11/12	0.91	0.09	72,85,96,98	0
2	OMZ	H	6	14/15	0.91	0.11	63,74,87,108	0
3	F93	J	6	14/15	0.91	0.15	54,62,80,109	0
2	D4P	F	4	11/12	0.91	0.11	71,75,93,95	0
3	D4P	I	5	11/12	0.92	0.09	57,64,72,82	0
3	F93	I	6	14/15	0.92	0.12	56,72,88,111	0
2	D3P	H	7	12/13	0.93	0.08	55,70,82,91	0
3	D4P	I	4	11/12	0.93	0.09	43,51,72,92	0
3	D4P	J	5	11/12	0.94	0.09	46,48,66,77	0
3	D3P	J	7	12/13	0.94	0.11	50,61,75,76	0
3	D4P	J	4	11/12	0.95	0.08	36,51,66,86	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

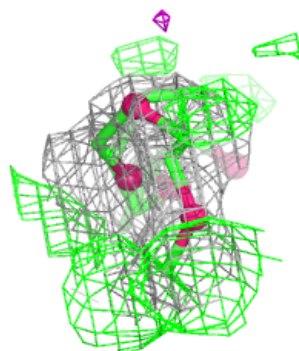
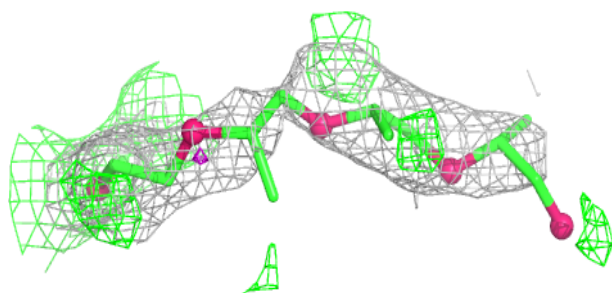
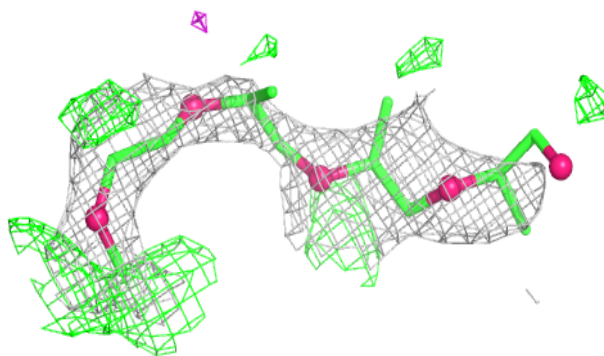
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MAN	G	103	11/12	0.52	0.15	95,121,134,145	0
7	MAN	H	103	11/12	0.72	0.15	94,98,108,117	0
4	JEF	A	801	17/41	0.73	0.30	69,85,113,115	0
7	MAN	F	103	11/12	0.82	0.13	87,102,107,108	0
5	F8F	H	101	12/13	0.83	0.14	84,101,113,118	0
9	WOO	J	103	11/12	0.83	0.18	68,77,95,103	0
5	F8F	G	101	12/13	0.84	0.11	89,96,107,115	0
9	WOO	I	103	11/12	0.84	0.16	80,85,111,112	0
4	JEF	B	802	17/41	0.84	0.26	57,92,101,103	0
5	F8F	F	101	12/13	0.85	0.14	89,105,115,116	0
4	JEF	A	802	17/41	0.85	0.22	76,101,117,122	0
4	JEF	C	801	17/41	0.87	0.20	52,80,100,102	0
8	F8X	J	102	12/13	0.87	0.12	62,72,82,89	0
4	JEF	C	802	17/41	0.89	0.22	59,85,102,105	0
4	JEF	B	801	17/41	0.89	0.19	68,96,103,105	0
8	F8X	I	102	12/13	0.90	0.08	62,78,89,93	0
6	M12	H	102	13/14	0.95	0.13	43,53,84,89	0
6	M12	G	102	13/14	0.95	0.16	54,69,91,93	0
6	M12	I	101	13/14	0.96	0.12	60,70,78,78	0
6	M12	J	101	13/14	0.96	0.17	63,67,75,76	0
6	M12	F	102	13/14	0.96	0.14	60,69,87,88	0

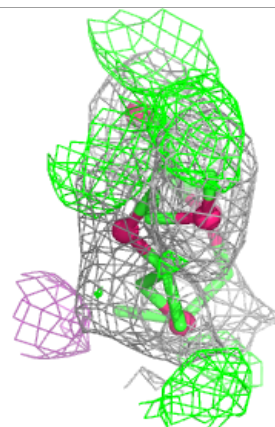
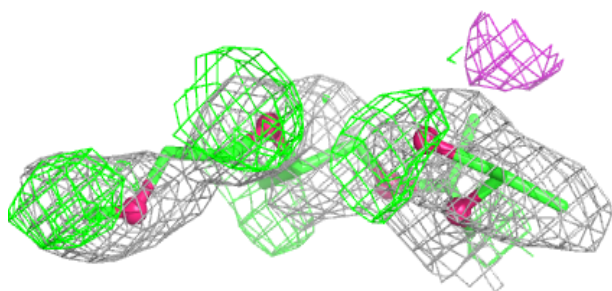
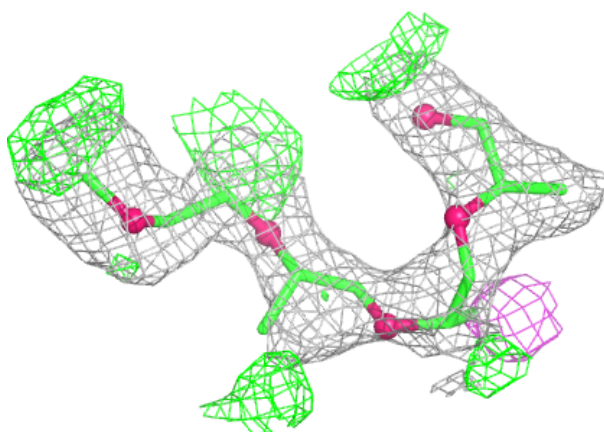
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JEF 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)

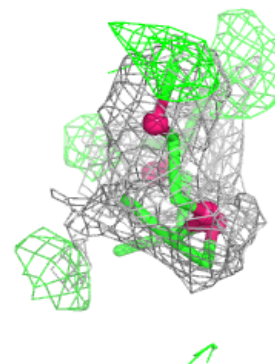
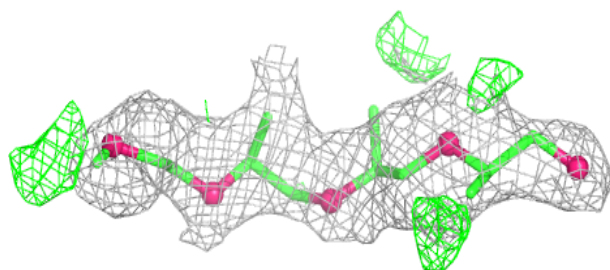
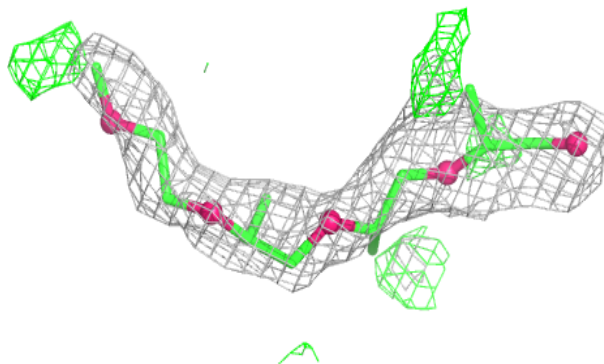
**Electron density around JEF B 802:**

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

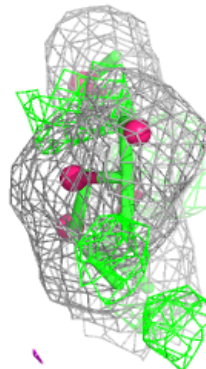
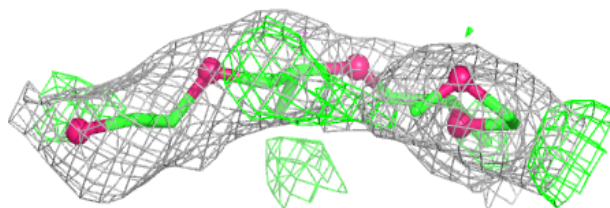
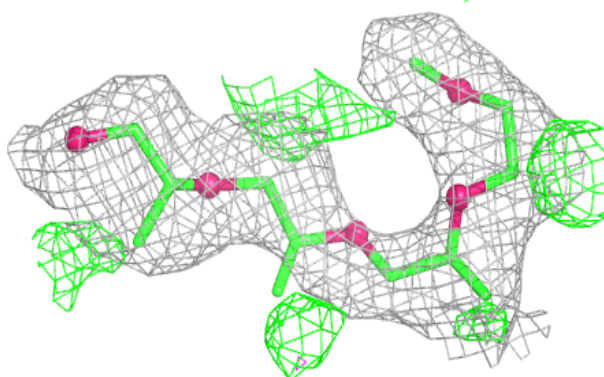


Electron density around JEF A 802:

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

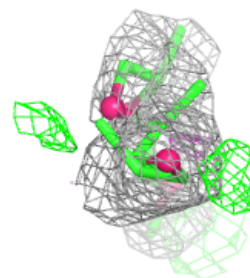
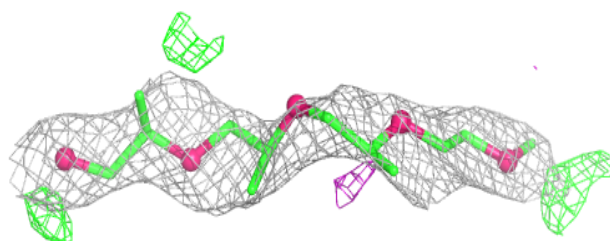
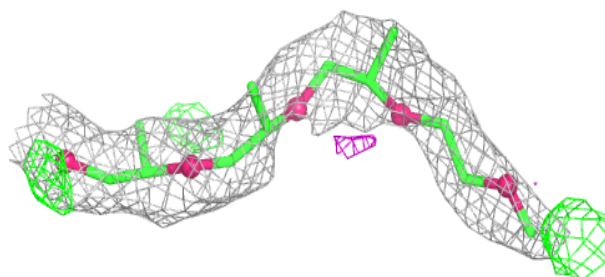
**Electron density around JEF C 801:**

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

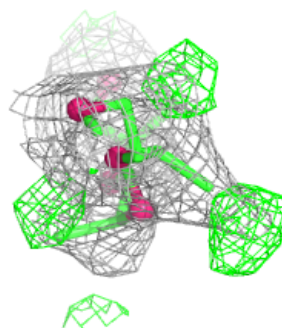
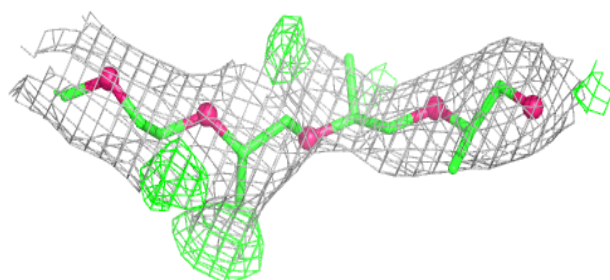
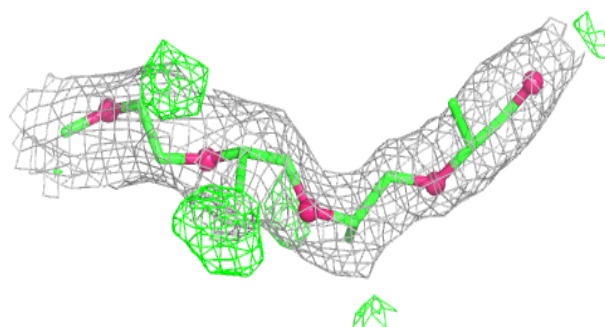


Electron density around JEF C 802:

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

**Electron density around JEF 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.