



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 8, 2020 – 02:12 PM JST

PDB ID : 6M5E
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

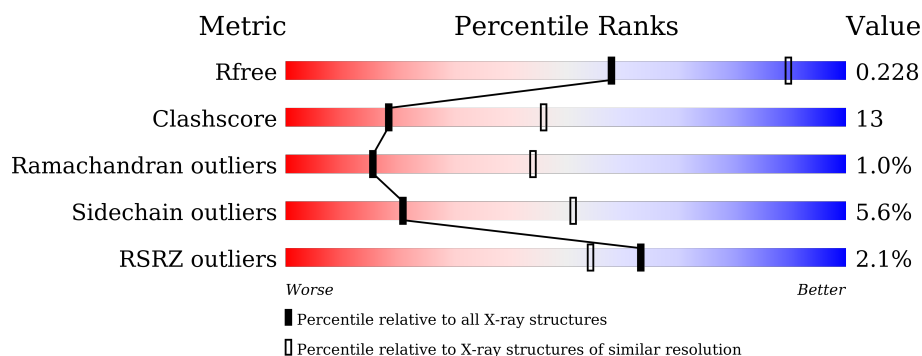
1 Overall quality at a glance

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>%</div> <div> <div>77%</div> <div>20%</div> <div>..</div> </div> </div>
1	B	585	<div> <div>5%</div> <div> <div>71%</div> <div>25%</div> <div>..</div> </div> </div>
1	C	585	<div> <div>76%</div> <div>20%</div> <div>..</div> </div>
2	F	8	<div> <div>25%</div> <div>25%</div> <div>50%</div> </div>
2	G	8	<div> <div>25%</div> <div>25%</div> <div>50%</div> </div>
2	H	8	<div> <div>25%</div> <div>50%</div> <div>25%</div> </div>

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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			

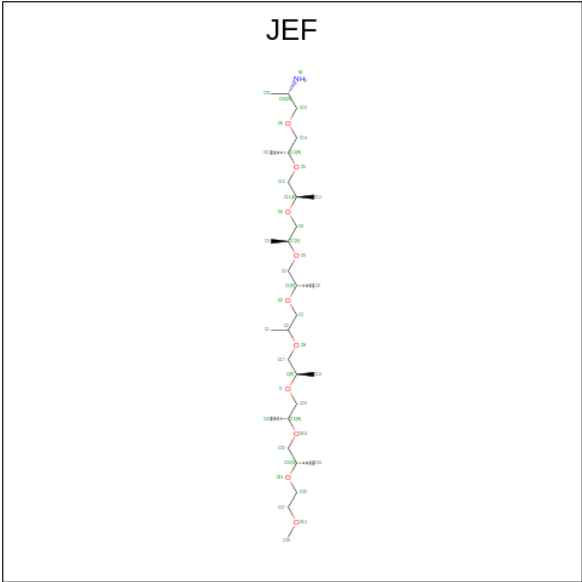
- Molecule 2 is a protein called dalbavancin.

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.

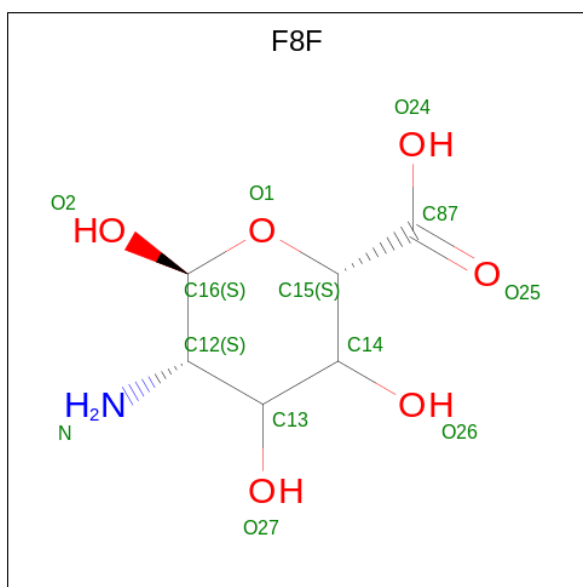
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	8	Total	C	Cl	N	O	0	0	0
			92	64	2	9	17			
3	J	8	Total	C	Cl	N	O	0	0	0
			92	64	2	9	17			

- Molecule 4 is O-(O-(2-AMINOPROPYL)-O'-(2-METHOXYETHYL)POLYPROPYLENE GLYCOL 500) (three-letter code: JEF) (formula: C₃₀H₆₃NO₁₀).



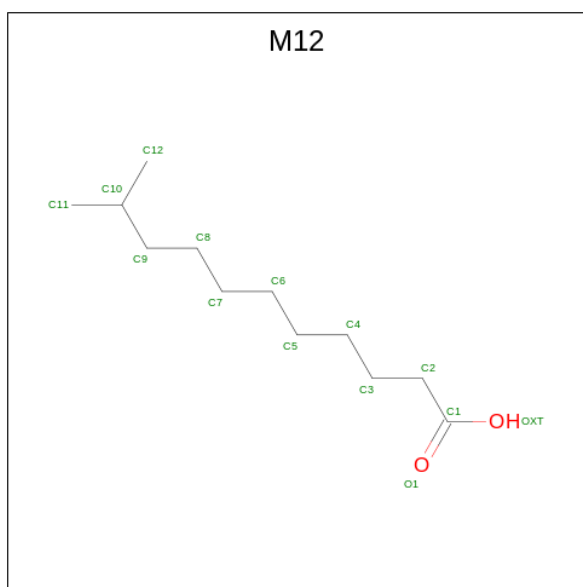
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			17	12	5		
4	A	1	Total	C	O	0	0
			17	12	5		
4	B	1	Total	C	O	0	0
			17	12	5		
4	B	1	Total	C	O	0	0
			17	12	5		
4	C	1	Total	C	O	0	0
			17	12	5		
4	C	1	Total	C	O	0	0
			17	12	5		

- Molecule 5 is (2S,5S)-5-azanyl-3,4,6-tris(oxidanyl)oxane-2-carboxylic acid (three-letter code: 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 (three-letter code: M12) (formula: $C_{12}H_{24}O_2$).



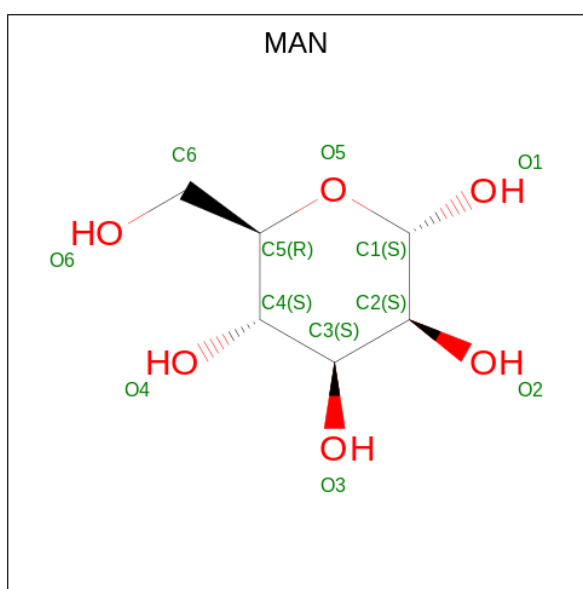
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	C	O	0	0
			13	12	1		

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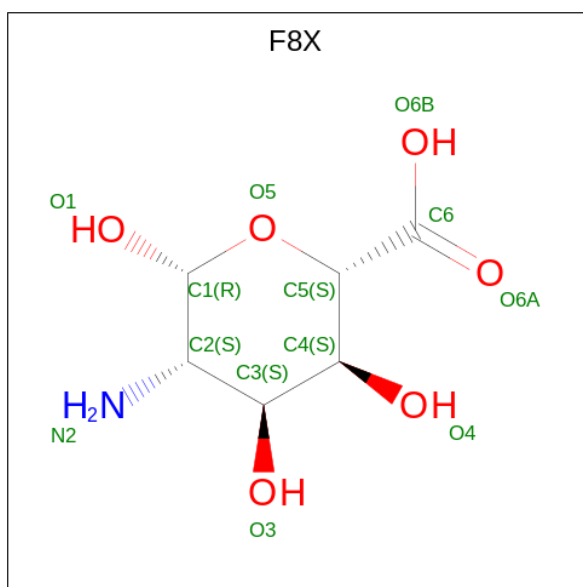
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	C	O	0	0
			13	12	1		
6	H	1	Total	C	O	0	0
			13	12	1		
6	I	1	Total	C	O	0	0
			13	12	1		
6	J	1	Total	C	O	0	0
			13	12	1		

- Molecule 7 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



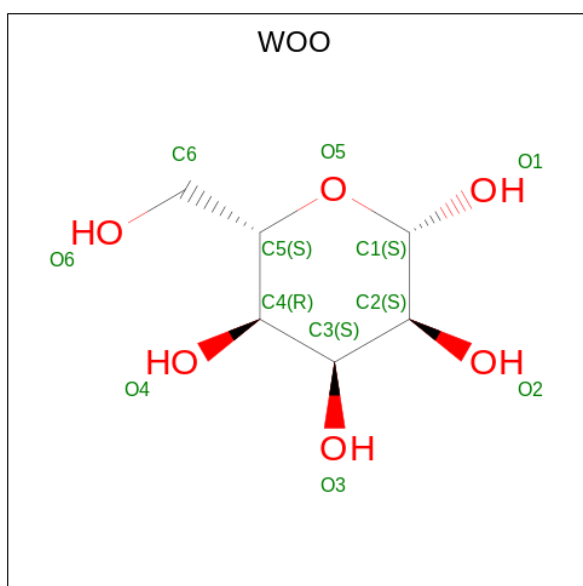
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total	C	O	0	0
			11	6	5		
7	G	1	Total	C	O	0	0
			11	6	5		
7	H	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is 2-amino-2-deoxy-beta-D-altropyranuronic acid (three-letter code: F8X) (formula: C₆H₁₁NO₆).



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 (three-letter code: 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		

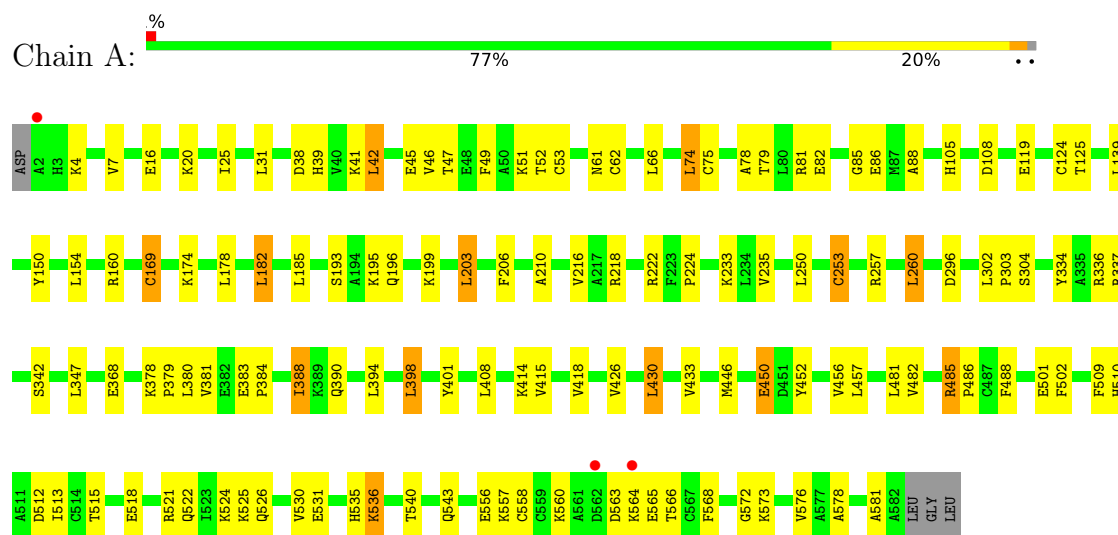
- Molecule 10 is water.

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

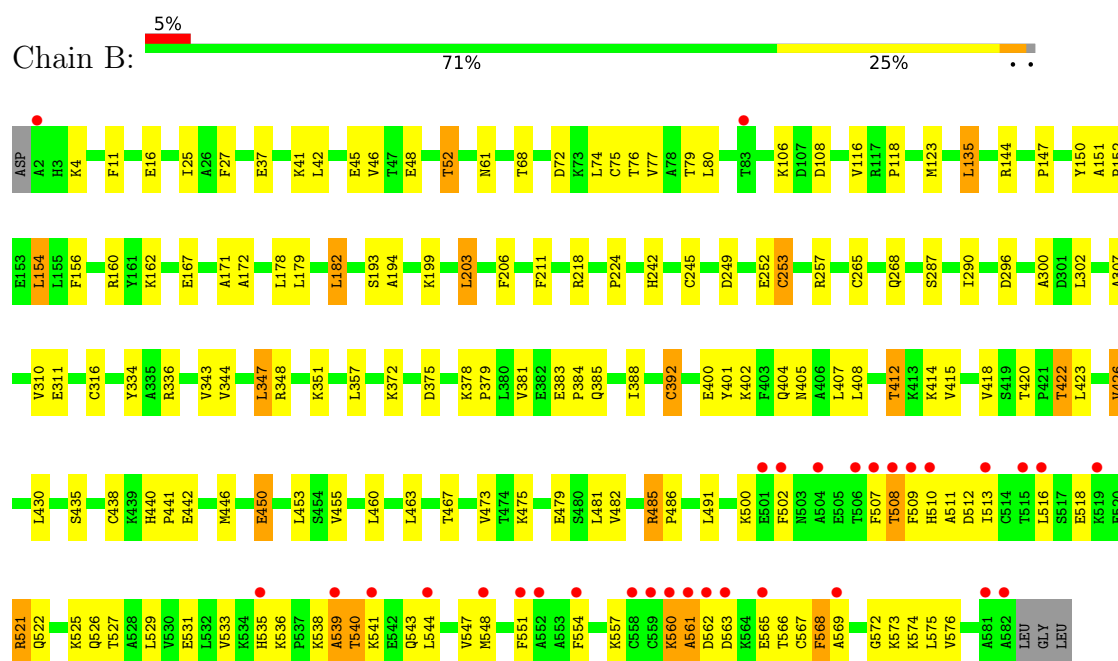
3 Residue-property plots [i](#)

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: Serum albumin

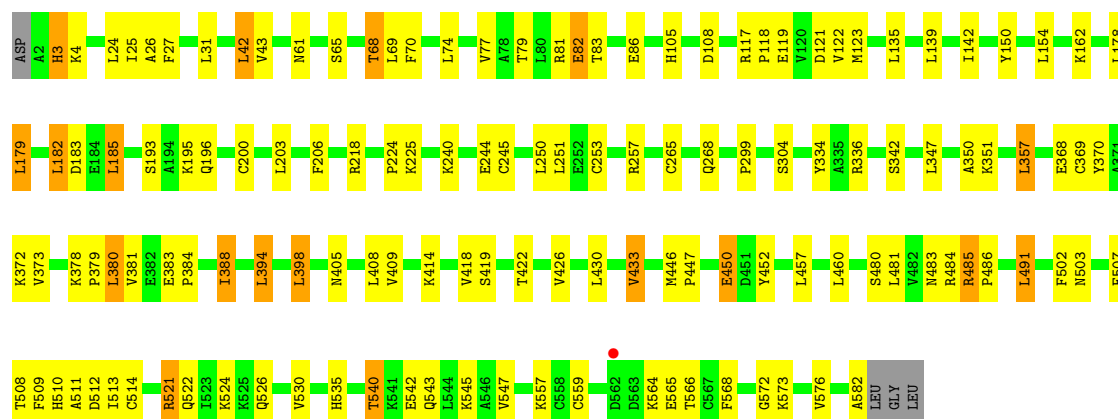


• Molecule 1: Serum albumin



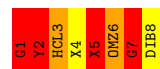
• Molecule 1: Serum albumin

Chain C:  76% 20% ..




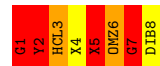
- Molecule 2: dalbavancin

Chain F:  25% 25% 50%



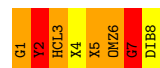
- Molecule 2: dalbavancin

Chain G:  25% 25% 50%




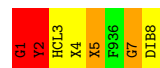
- Molecule 2: dalbavancin

Chain H:  25% 50% 25%



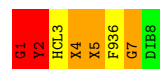
- Molecule 3: dalbavancin

Chain I:  13% 38% 25% 25%



- Molecule 3: dalbavancin

Chain J:  13% 25% 38% 25%



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 49.26 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.78-2.80) 100.0 (49.26-2.80)	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 0.180 , 0.228	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 , 43.2	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: D4P, F8X, 5PG, DIB, F93, WOO, M12, JEF, D3P, OMZ, F8F, HCL, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.52	1/4707 (0.0%)	0.72	4/6350 (0.1%)
1	B	0.53	2/4694 (0.0%)	0.67	5/6337 (0.1%)
1	C	0.56	2/4708 (0.0%)	0.71	7/6351 (0.1%)
2	F	0.44	0/12	1.30	0/15
2	G	0.40	0/12	1.39	0/15
2	H	0.38	0/12	1.14	0/15
3	I	0.46	0/12	0.79	0/15
3	J	0.43	0/12	0.84	0/15
All	All	0.54	5/14169 (0.0%)	0.70	16/19113 (0.1%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	253	CYS	CB-SG	-9.45	1.66	1.82
1	B	316	CYS	CB-SG	-7.94	1.68	1.82
1	C	253	CYS	CB-SG	-6.42	1.71	1.82
1	C	200	CYS	CB-SG	-5.10	1.73	1.81
1	A	253	CYS	CB-SG	-5.05	1.73	1.81

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	CYS	CA-CB-SG	-10.23	95.58	114.00
1	A	62	CYS	CA-CB-SG	-10.09	95.84	114.00
1	A	169	CYS	CA-CB-SG	-7.99	99.62	114.00
1	B	316	CYS	CA-CB-SG	-6.65	102.03	114.00
1	C	42	LEU	CA-CB-CG	6.52	130.30	115.30

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	Sidechain,Peptide
2	F	5	D4P	Mainchain,Peptide
2	F	7	D3P	Peptide
2	G	1	5PG	Peptide

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	4618	0	4529	96	0
1	B	4604	0	4499	127	0
1	C	4618	0	4534	113	0
2	F	92	0	46	7	0
2	G	92	0	44	7	0
2	H	92	0	43	6	0
3	I	92	0	43	10	0
3	J	92	0	42	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	14095	382	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 13.

The worst 5 of 382 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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	579/585 (99%)	559 (96%)	20 (4%)	0	100	100
1	B	579/585 (99%)	547 (94%)	23 (4%)	9 (2%)	9	31
1	C	579/585 (99%)	560 (97%)	15 (3%)	4 (1%)	22	53
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%)	15	44

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

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	507/511 (99%)	481 (95%)	26 (5%)	24	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	503/511 (98%)	476 (95%)	27 (5%)	22	53
1	C	507/511 (99%)	480 (95%)	27 (5%)	22	54
2	F	1/1 (100%)	0	1 (100%)	0	0
2	G	1/1 (100%)	0	1 (100%)	0	0
2	H	1/1 (100%)	0	1 (100%)	0	0
3	I	1/1 (100%)	0	1 (100%)	0	0
3	J	1/1 (100%)	0	1 (100%)	0	0
All	All	1522/1538 (99%)	1437 (94%)	85 (6%)	21	51

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	392	CYS
1	B	467	THR
1	C	521	ARG
1	B	412	THR
1	B	438	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	C	3	HIS
1	C	9	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	$\# Z > 2$
3	F93	I	6	3	12,14,15	0.58	0	17,19,21	0.68	0
3	5PG	J	1	3	12,12,13	0.84	1 (8%)	11,15,17	0.42	0
2	OMZ	H	6	2	12,14,15	0.42	0	17,19,21	2.38	3 (17%)
3	F93	J	6	3	12,14,15	0.51	0	17,19,21	0.76	0
2	OMZ	F	6	2	12,14,15	0.53	0	17,19,21	2.40	3 (17%)
3	HCL	I	3	3	12,13,14	0.77	0	13,18,20	1.85	1 (7%)
2	HCL	F	3	2	12,13,14	1.27	1 (8%)	13,18,20	2.19	3 (23%)
2	D4P	G	5	2	10,11,12	1.08	1 (10%)	11,14,16	0.86	0
3	D3P	I	7	3	11,12,13	0.77	0	13,16,18	2.35	3 (23%)
3	HCL	J	3	3	12,13,14	0.88	1 (8%)	13,18,20	2.05	1 (7%)
3	D4P	J	5	3	10,11,12	0.66	0	11,14,16	0.86	0
2	5PG	F	1	2	12,12,13	0.92	1 (8%)	11,15,17	0.98	0
3	5PG	I	1	3	12,12,13	0.77	1 (8%)	11,15,17	0.43	0
3	D4P	I	4	3	10,11,12	0.69	0	11,14,16	0.68	0
2	D3P	F	7	2	11,12,13	0.78	0	13,16,18	1.91	4 (30%)
2	D3P	H	7	2	11,12,13	0.84	0	13,16,18	2.02	4 (30%)
2	D4P	F	5	2	10,11,12	1.43	1 (10%)	11,14,16	0.84	0
2	OMZ	G	6	2	12,14,15	0.48	0	17,19,21	2.36	3 (17%)
2	5PG	G	1	2	12,12,13	0.57	0	11,15,17	1.02	1 (9%)
2	D4P	H	4	2,5	10,11,12	0.73	0	11,14,16	0.87	1 (9%)
3	D4P	I	5	3	10,11,12	0.72	0	11,14,16	0.79	0
2	HCL	G	3	2	12,13,14	1.21	1 (8%)	13,18,20	1.99	2 (15%)
3	D4P	J	4	3	10,11,12	1.08	1 (10%)	11,14,16	0.67	0
2	D4P	G	4	2,5	10,11,12	1.14	1 (10%)	11,14,16	0.82	1 (9%)
3	D3P	J	7	3	11,12,13	0.77	0	13,16,18	2.31	3 (23%)
2	D4P	H	5	2	10,11,12	0.84	0	11,14,16	0.82	0
2	D3P	G	7	2	11,12,13	0.85	0	13,16,18	2.25	4 (30%)
2	D4P	F	4	2,5	10,11,12	0.78	0	11,14,16	0.98	1 (9%)
2	HCL	H	3	2	12,13,14	0.98	1 (8%)	13,18,20	2.20	2 (15%)
2	5PG	H	1	2	12,12,13	0.58	0	11,15,17	0.96	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
3	F93	J	6	3	-	5/9/10/12	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
2	D4P	H	4	2,5	1/1/1/2	4/4/6/8	0/1/1/1
2	D4P	F	4	2,5	1/1/1/2	4/4/6/8	0/1/1/1
2	D3P	H	7	2	1/1/1/2	2/4/6/8	0/1/1/1
3	HCL	I	3	3	-	3/3/6/8	0/1/1/1
2	HCL	F	3	2	-	0/3/6/8	0/1/1/1
2	D4P	G	5	2	-	0/4/6/8	0/1/1/1
3	D3P	I	7	3	-	0/4/6/8	0/1/1/1
3	HCL	J	3	3	-	3/3/6/8	0/1/1/1
3	D4P	J	5	3	-	0/4/6/8	0/1/1/1
2	5PG	F	1	2	1/1/1/3	1/5/8/10	0/1/1/1
3	5PG	I	1	3	-	0/5/8/10	0/1/1/1
3	D4P	I	4	3	-	2/4/6/8	0/1/1/1
2	D3P	F	7	2	1/1/1/2	2/4/6/8	0/1/1/1
2	D4P	F	5	2	-	0/4/6/8	0/1/1/1
2	OMZ	G	6	2	1/1/2/3	4/9/10/12	0/1/1/1
2	5PG	G	1	2	1/1/1/3	1/5/8/10	0/1/1/1
2	OMZ	H	6	2	1/1/2/3	4/9/10/12	0/1/1/1
3	D4P	I	5	3	-	0/4/6/8	0/1/1/1
2	HCL	G	3	2	-	0/3/6/8	0/1/1/1
3	D4P	J	4	3	-	2/4/6/8	0/1/1/1
2	D4P	G	4	2,5	1/1/1/2	4/4/6/8	0/1/1/1
3	D3P	J	7	3	-	0/4/6/8	0/1/1/1
2	D4P	H	5	2	-	0/4/6/8	0/1/1/1
2	D3P	G	7	2	1/1/1/2	2/4/6/8	0/1/1/1
2	OMZ	F	6	2	1/1/2/3	4/9/10/12	0/1/1/1
2	HCL	H	3	2	-	0/3/6/8	0/1/1/1
2	5PG	H	1	2	1/1/1/3	1/5/8/10	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	5	D4P	CA-C	4.04	1.59	1.51
2	F	3	HCL	CA-C	3.89	1.59	1.51
2	G	3	HCL	CA-C	3.58	1.58	1.51
2	G	4	D4P	CA-C	3.22	1.57	1.51
3	J	4	D4P	CA-C	-3.18	1.44	1.51

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	6	OMZ	OC-CB-CA	7.85	123.85	107.28
2	F	6	OMZ	OC-CB-CA	7.70	123.53	107.28
2	G	6	OMZ	OC-CB-CA	7.34	122.76	107.28
3	J	3	HCL	C1-CA-N	7.20	129.24	112.10
2	H	3	HCL	C1-CA-N	7.15	129.13	112.10

5 of 12 chirality outliers are listed below:

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

5 of 53 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	6	F93	C-CA-CB-CG
3	I	6	F93	N-CA-CB-CG
3	I	6	F93	C-CA-CB-OC
3	I	6	F93	N-CA-CB-OC
3	I	6	F93	O-C-CA-CB

There are no ring outliers.

24 monomers are involved in 39 short contacts:

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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$
4	JEF	A	802	-	13,16,40	0.31	0	15,18,48	0.92	0
5	F8F	F	101	2,6	9,12,13	0.97	1 (11%)	9,17,19	4.97	6 (66%)
8	F8X	J	102	6	9,12,13	0.78	0	9,17,19	1.03	0
6	M12	J	101	8	12,12,13	0.23	0	12,12,14	0.34	0
6	M12	F	102	5	12,12,13	0.31	0	12,12,14	0.25	0
8	F8X	I	102	6	9,12,13	0.81	0	9,17,19	0.75	0
7	MAN	G	103	-	11,11,12	0.58	0	15,15,17	3.79	9 (60%)
6	M12	I	101	8	12,12,13	0.28	0	12,12,14	0.35	0
4	JEF	C	802	-	13,16,40	0.35	0	15,18,48	1.00	0
6	M12	G	102	5	12,12,13	0.28	0	12,12,14	0.27	0
5	F8F	G	101	2,6	9,12,13	0.86	1 (11%)	9,17,19	5.17	6 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	JEF	B	802	-	13,16,40	0.35	0	15,18,48	0.85	0
7	MAN	F	103	-	11,11,12	0.55	0	15,15,17	3.96	9 (60%)
9	WOO	I	103	-	11,11,12	0.66	0	15,15,17	1.12	3 (20%)
7	MAN	H	103	-	11,11,12	0.50	0	15,15,17	3.87	9 (60%)
4	JEF	C	801	-	13,16,40	0.39	0	15,18,48	0.88	0
4	JEF	B	801	-	13,16,40	0.29	0	15,18,48	1.05	1 (6%)
4	JEF	A	801	-	13,16,40	0.55	0	15,18,48	1.11	2 (13%)
6	M12	H	102	5	12,12,13	0.32	0	12,12,14	0.33	0
5	F8F	H	101	2,6	9,12,13	0.85	1 (11%)	9,17,19	5.11	6 (66%)
9	WOO	J	103	-	11,11,12	0.69	0	15,15,17	0.99	1 (6%)

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	F8F	F	101	2,6	3/3/5/6	0/0/21/24	0/1/1/1
4	JEF	A	802	-	-	8/17/17/46	-
8	F8X	J	102	6	-	0/0/21/24	0/1/1/1
6	M12	J	101	8	-	3/9/10/11	-
6	M12	F	102	5	-	4/9/10/11	-
8	F8X	I	102	6	-	0/0/21/24	0/1/1/1
7	MAN	G	103	-	-	2/2/19/22	0/1/1/1
6	M12	I	101	8	-	6/9/10/11	-
5	F8F	H	101	2,6	3/3/5/6	0/0/21/24	0/1/1/1
6	M12	G	102	5	-	4/9/10/11	-
5	F8F	G	101	2,6	4/4/5/6	0/0/21/24	0/1/1/1
4	JEF	B	802	-	-	5/17/17/46	-
7	MAN	F	103	-	-	1/2/19/22	0/1/1/1
9	WOO	I	103	-	-	2/2/19/22	0/1/1/1
7	MAN	H	103	-	-	1/2/19/22	0/1/1/1
4	JEF	C	801	-	-	7/17/17/46	-
4	JEF	B	801	-	-	5/17/17/46	-
4	JEF	A	801	-	-	7/17/17/46	-
6	M12	H	102	5	-	4/9/10/11	-
4	JEF	C	802	-	-	7/17/17/46	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	WOO	J	103	-	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	101	F8F	C16-C12	2.64	1.55	1.52
5	G	101	F8F	C16-C12	2.39	1.55	1.52
5	H	101	F8F	C16-C12	2.31	1.55	1.52

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	10.20	129.54	110.05
5	H	101	F8F	O26-C14-C15	9.96	129.09	110.05
5	F	101	F8F	O26-C14-C15	9.27	127.76	110.05
5	F	101	F8F	O27-C13-C12	7.80	124.10	109.81
5	H	101	F8F	O27-C13-C12	7.70	123.92	109.81

5 of 10 chirality outliers are listed below:

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

5 of 66 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	802	JEF	O10-C32-C33-O11
4	A	802	JEF	O-C-C17-OH
4	C	802	JEF	C40-C19-O10-C32
4	C	802	JEF	O10-C19-C20-O
4	C	802	JEF	C40-C19-C20-O

There are no ring outliers.

16 monomers are involved in 55 short contacts:

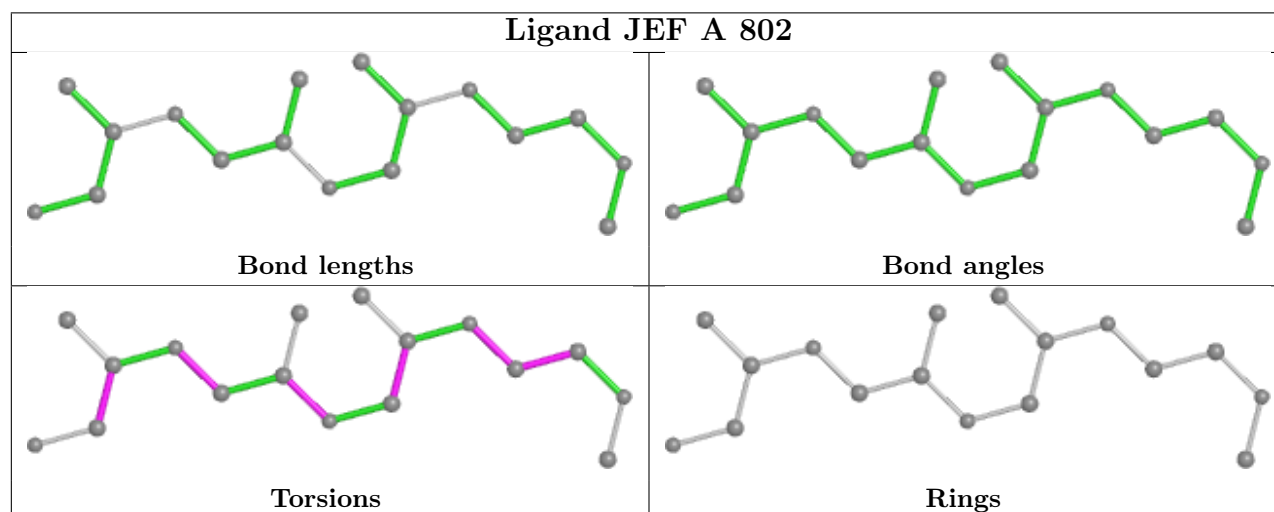
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	802	JEF	3	0

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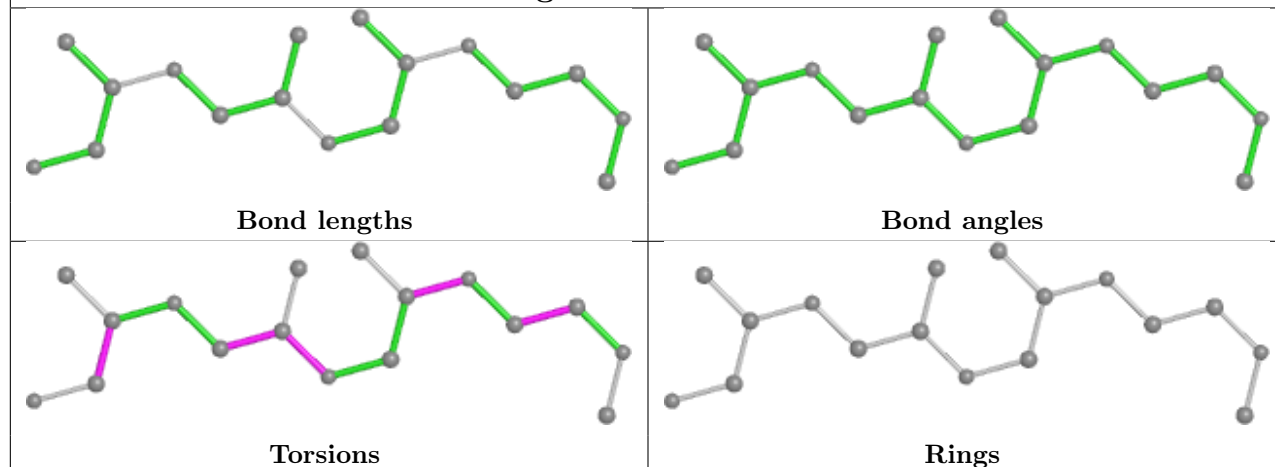
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	102	M12	2	0
8	I	102	F8X	1	0
7	G	103	MAN	1	0
6	I	101	M12	1	0
4	C	802	JEF	5	0
6	G	102	M12	2	0
4	B	802	JEF	9	0
7	F	103	MAN	1	0
9	I	103	WOO	2	0
7	H	103	MAN	1	0
4	C	801	JEF	10	0
4	B	801	JEF	3	0
4	A	801	JEF	10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

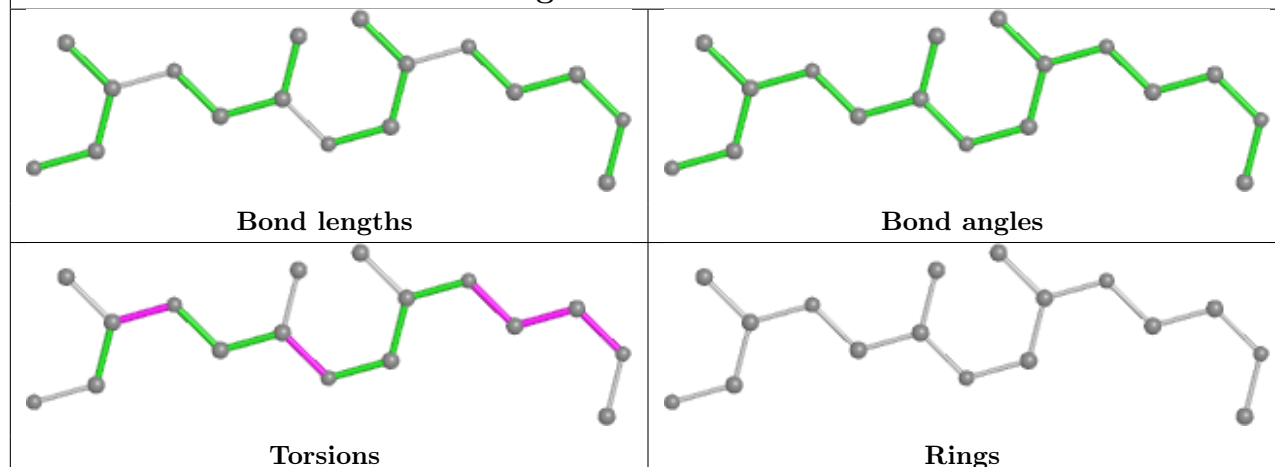
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



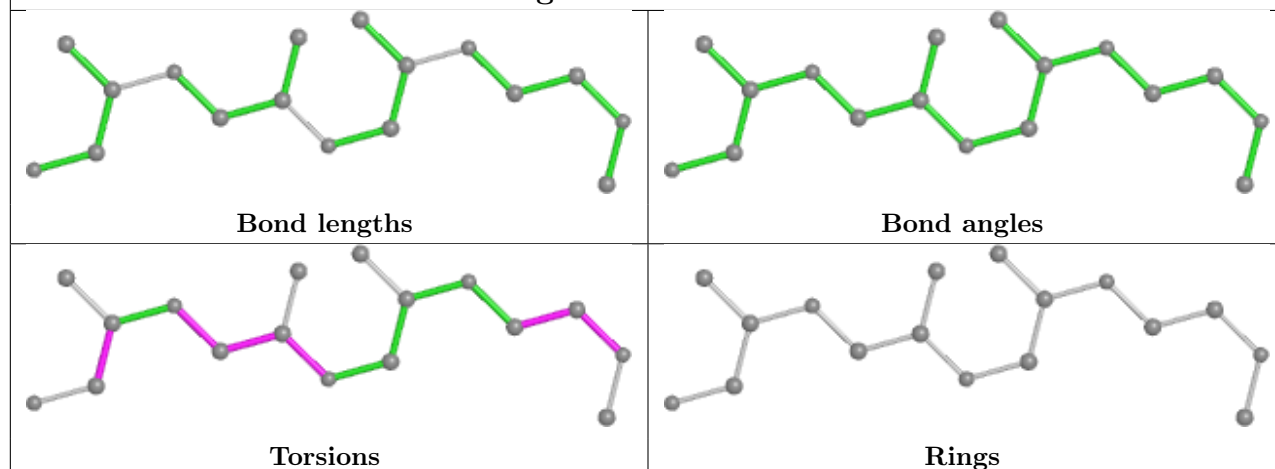
Ligand JEF C 802

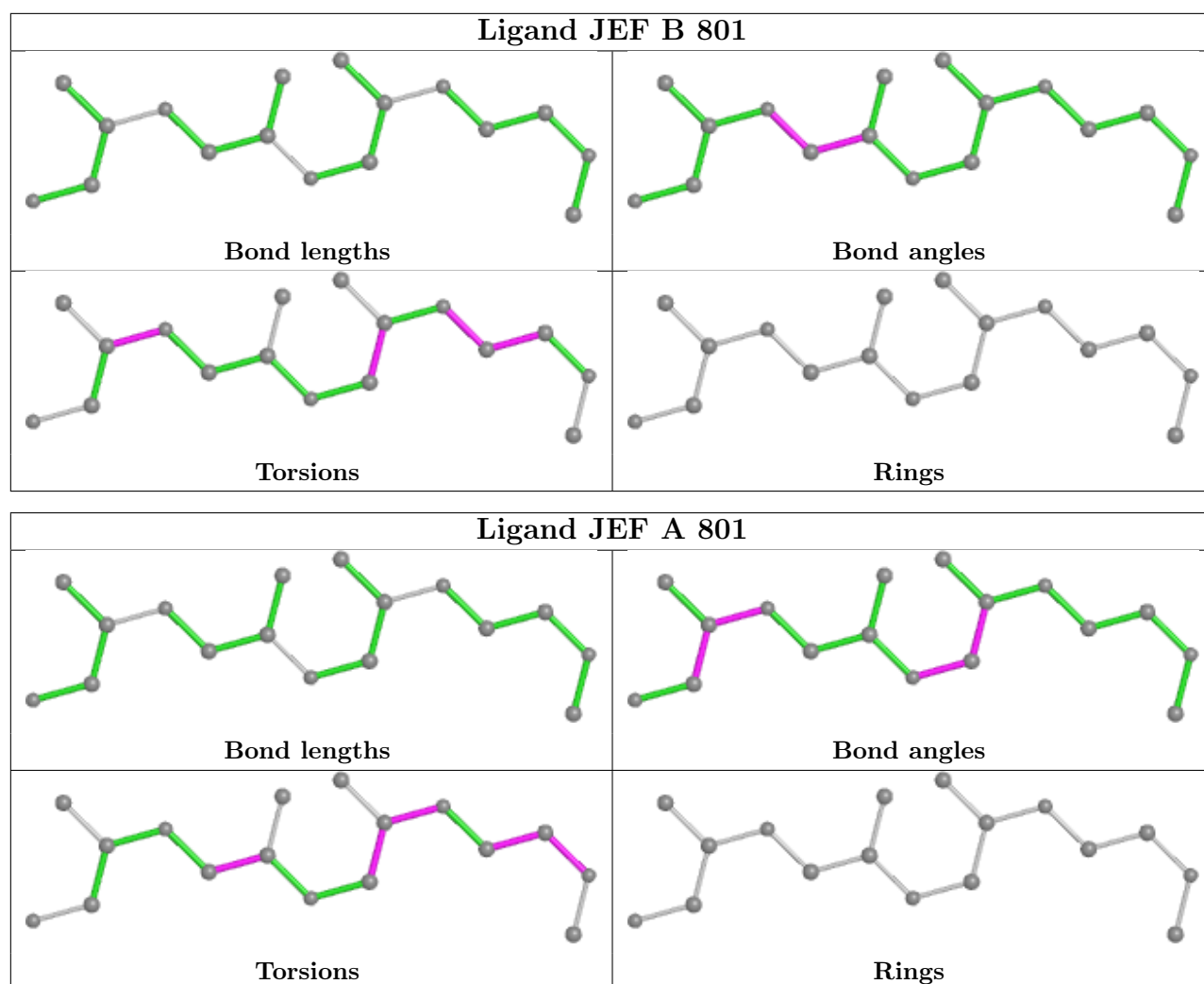


Ligand JEF B 802



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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	581/585 (99%)	-0.53	3 (0%) 91 88	32, 54, 99, 190	0
1	B	581/585 (99%)	-0.17	32 (5%) 25 16	29, 59, 174, 221	0
1	C	581/585 (99%)	-0.51	1 (0%) 95 94	29, 50, 95, 141	0
2	F	1/8 (12%)	-0.69	0 100 100	92, 92, 92, 92	0
2	G	1/8 (12%)	-0.24	0 100 100	101, 101, 101, 101	0
2	H	1/8 (12%)	0.01	0 100 100	83, 83, 83, 83	0
3	I	1/8 (12%)	-0.24	0 100 100	73, 73, 73, 73	0
3	J	1/8 (12%)	-0.05	0 100 100	64, 64, 64, 64	0
All	All	1748/1795 (97%)	-0.40	36 (2%) 63 54	29, 54, 123, 221	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	516	LEU	4.7
1	B	563	ASP	4.6
1	B	507	PHE	4.4
1	B	562	ASP	4.2
1	B	551	PHE	4.0

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

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	HCL	G	3	13/14	0.78	0.22	98,107,118,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	HCL	F	3	13/14	0.80	0.23	92,106,127,143	0
2	D4P	G	5	11/12	0.83	0.20	71,91,99,100	0
2	5PG	G	1	12/13	0.84	0.25	102,110,115,116	0
3	5PG	J	1	12/13	0.84	0.20	67,87,107,127	0
2	D4P	G	4	11/12	0.86	0.19	93,103,109,113	0
2	HCL	H	3	13/14	0.86	0.24	83,98,125,143	0
2	D3P	G	7	12/13	0.87	0.20	60,82,103,123	0
3	5PG	I	1	12/13	0.89	0.27	83,96,115,120	0
2	OMZ	G	6	14/15	0.89	0.23	91,100,107,116	0
3	HCL	J	3	13/14	0.89	0.21	78,91,120,139	0
2	5PG	F	1	12/13	0.89	0.23	84,99,110,122	0
2	5PG	H	1	12/13	0.90	0.21	70,86,91,104	0
3	HCL	I	3	13/14	0.91	0.19	81,88,110,136	0
2	D4P	F	4	11/12	0.92	0.17	71,75,93,95	0
2	D4P	H	4	11/12	0.92	0.13	69,74,81,89	0
2	OMZ	F	6	14/15	0.92	0.20	79,83,96,128	0
2	D3P	F	7	12/13	0.93	0.14	69,86,100,102	0
2	D4P	F	5	11/12	0.93	0.18	72,85,96,98	0
3	F93	I	6	14/15	0.93	0.17	56,72,88,111	0
3	D3P	I	7	12/13	0.93	0.14	62,67,71,82	0
2	OMZ	H	6	14/15	0.94	0.15	63,74,87,108	0
3	F93	J	6	14/15	0.94	0.22	54,62,80,109	0
3	D4P	I	5	11/12	0.94	0.12	57,64,72,82	0
3	D4P	I	4	11/12	0.95	0.11	43,51,72,92	0
3	D3P	J	7	12/13	0.95	0.18	50,61,75,76	0
3	D4P	J	5	11/12	0.96	0.13	46,48,66,77	0
2	D3P	H	7	12/13	0.96	0.11	55,70,82,91	0
3	D4P	J	4	11/12	0.96	0.12	36,51,66,86	0
2	D4P	H	5	11/12	0.96	0.16	67,80,88,99	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

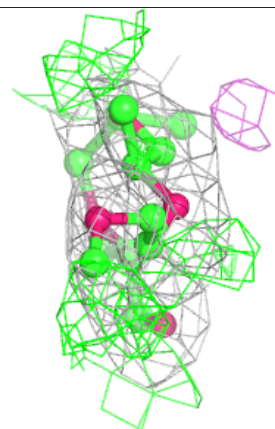
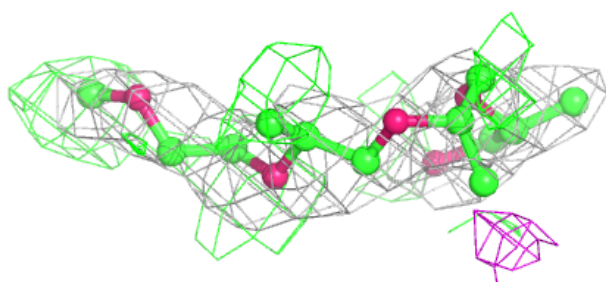
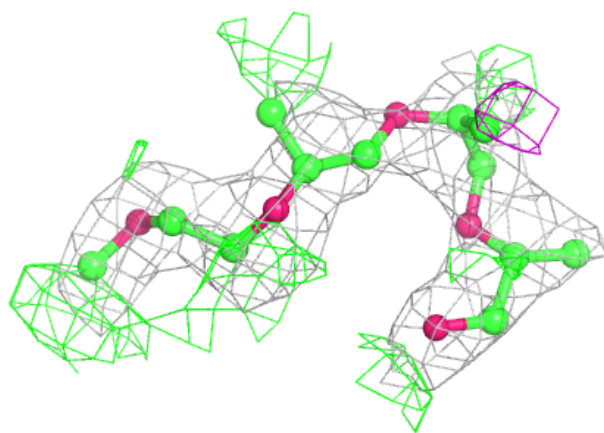
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	JEF	B	802	17/41	0.77	0.31	57,92,101,103	0
4	JEF	A	801	17/41	0.77	0.32	69,85,113,115	0
4	JEF	C	801	17/41	0.81	0.29	52,80,100,102	0
7	MAN	G	103	11/12	0.82	0.30	95,121,134,145	0
4	JEF	A	802	17/41	0.83	0.27	76,101,117,122	0
4	JEF	C	802	17/41	0.87	0.25	59,85,102,105	0
9	WOO	I	103	11/12	0.89	0.18	80,85,111,112	0
4	JEF	B	801	17/41	0.89	0.27	68,96,103,105	0
7	MAN	H	103	11/12	0.89	0.17	94,98,108,117	0
7	MAN	F	103	11/12	0.90	0.12	87,102,107,108	0
5	F8F	F	101	12/13	0.90	0.14	89,105,115,116	0
5	F8F	H	101	12/13	0.90	0.15	84,101,113,118	0
5	F8F	G	101	12/13	0.91	0.15	89,96,107,115	0
9	WOO	J	103	11/12	0.91	0.19	68,77,95,103	0
6	M12	G	102	13/14	0.92	0.33	54,69,91,93	0
6	M12	H	102	13/14	0.92	0.26	43,53,84,89	0
8	F8X	J	102	12/13	0.94	0.17	62,72,82,89	0
8	F8X	I	102	12/13	0.94	0.15	62,78,89,93	0
6	M12	F	102	13/14	0.95	0.27	60,69,87,88	0
6	M12	J	101	13/14	0.95	0.32	63,67,75,76	0
6	M12	I	101	13/14	0.96	0.34	60,70,78,78	0

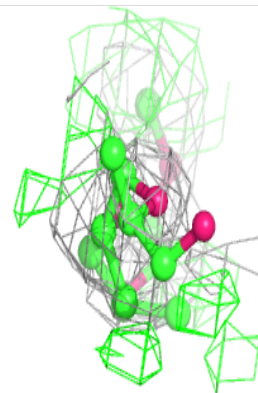
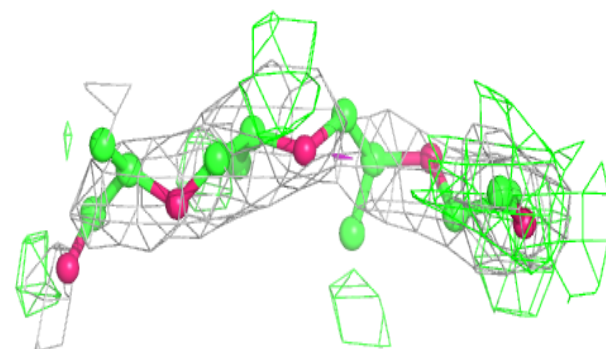
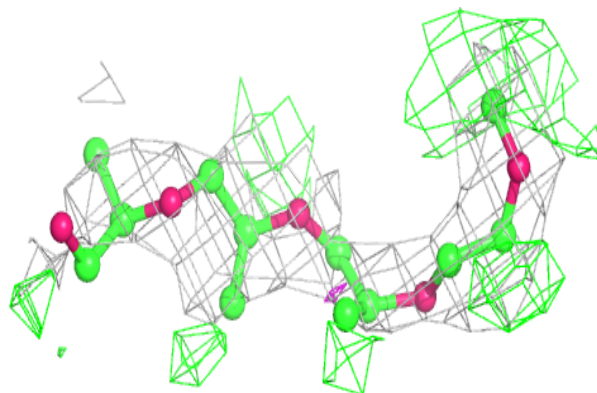
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JEF 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)

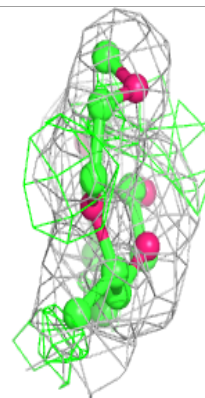
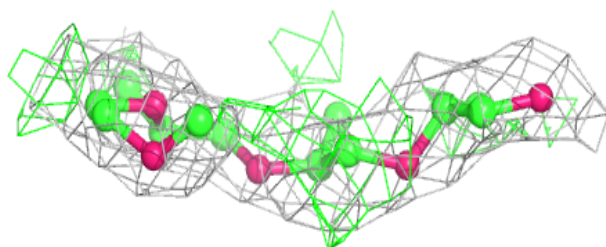
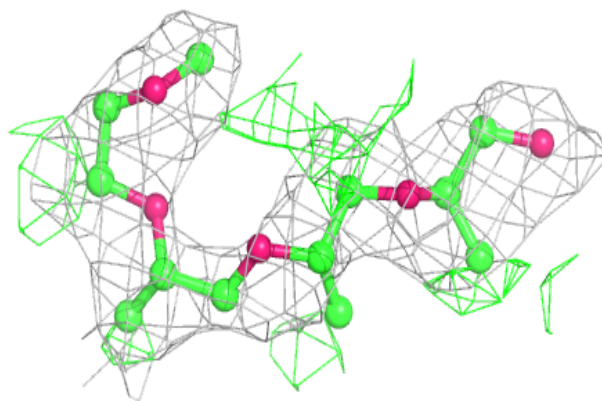
**Electron density around JEF A 801:**

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

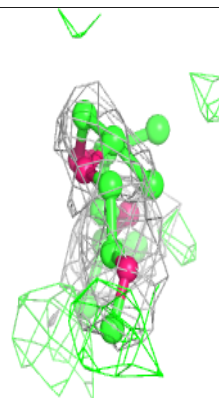
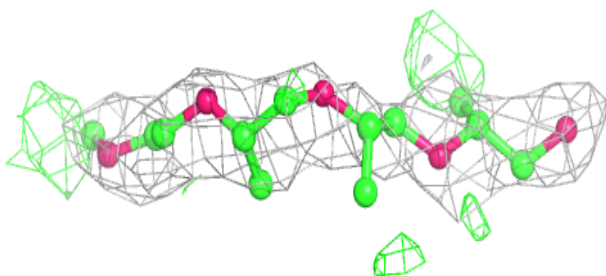
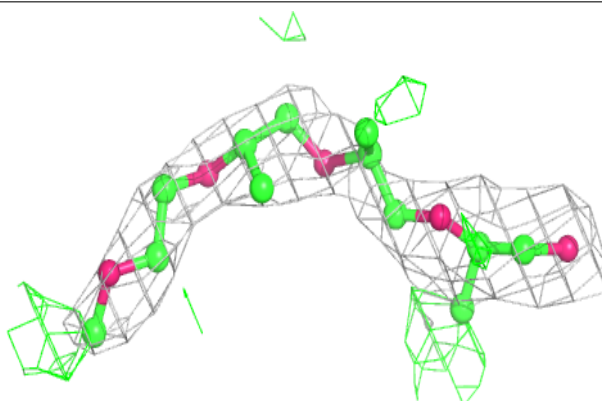


Electron density around JEF C 801:

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

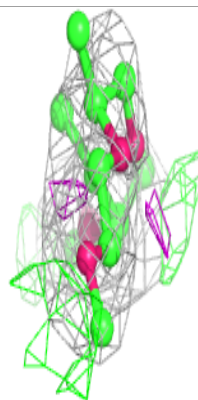
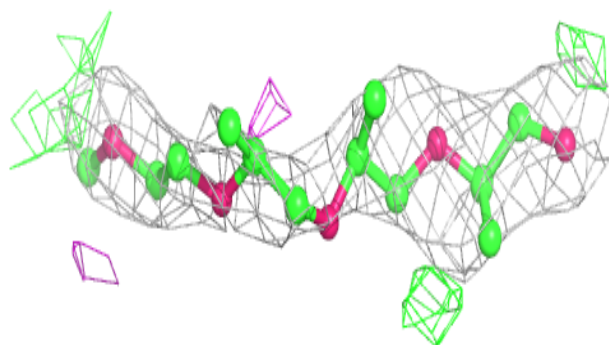
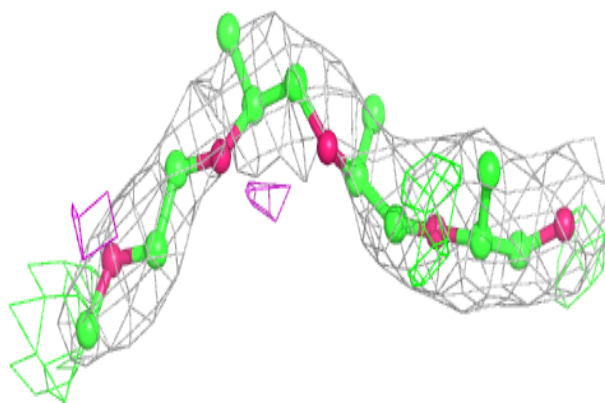
**Electron density around JEF A 802:**

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

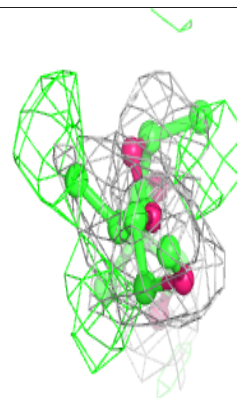
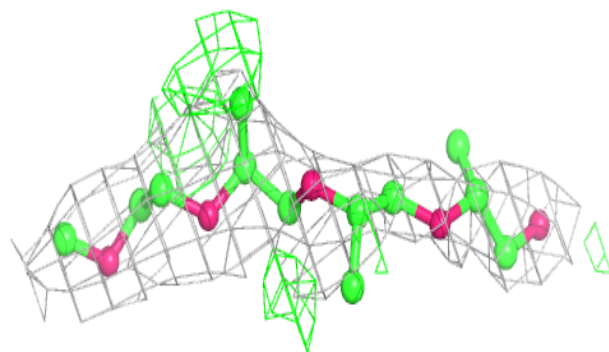
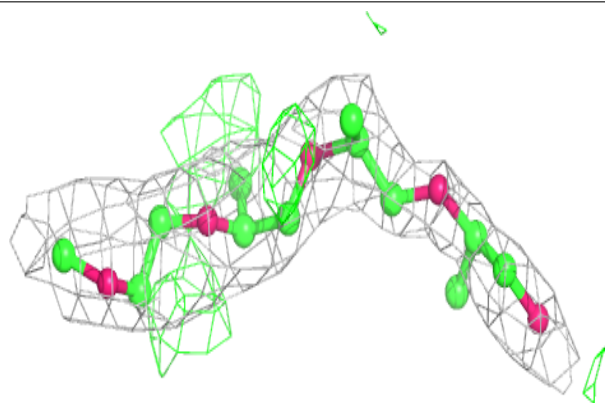


Electron density around JEF C 802:

$2mF_o-DF_c$ (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.