wwPDB X-ray Structure Validation Summary Report (i)

Jun 13, 2024 – 11:46 AM EDT

PDB ID	:	1PVJ
Title	:	Crystal structure of the Streptococcal pyrogenic exotoxin B (SpeB)- inhibitor complex
Authors	:	Ziomek, E.; Sivaraman, J.; Doran, J.; Menard, R.; Cygler, M.
Deposited on	:	2003-06-27
Resolution	:	3.00 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:

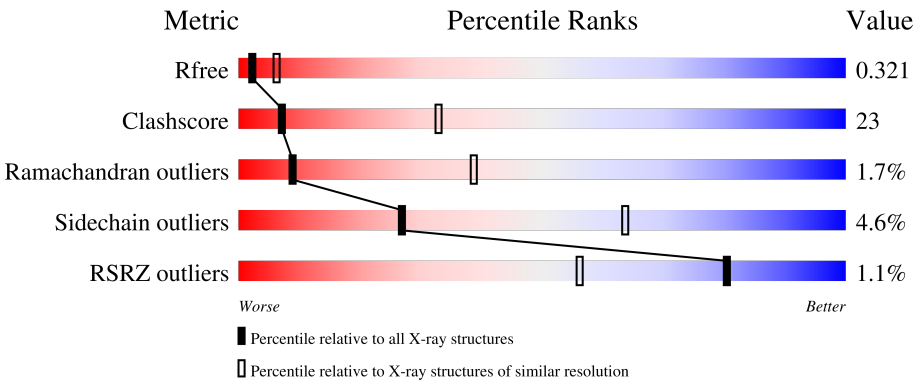
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	368	2%, 55%, 33%, •, 8%
1	B	368	59%, 29%, 5%, 8%
1	C	368	60%, 29%, •, 8%
1	D	368	2%, 54%, 34%, •, 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	ZFB	A	450	-	X	X	X
2	ZFB	B	450	-	X	X	X
2	ZFB	C	450	-	X	X	X
2	ZFB	D	450	-	X	X	-

2 Entry composition (i)

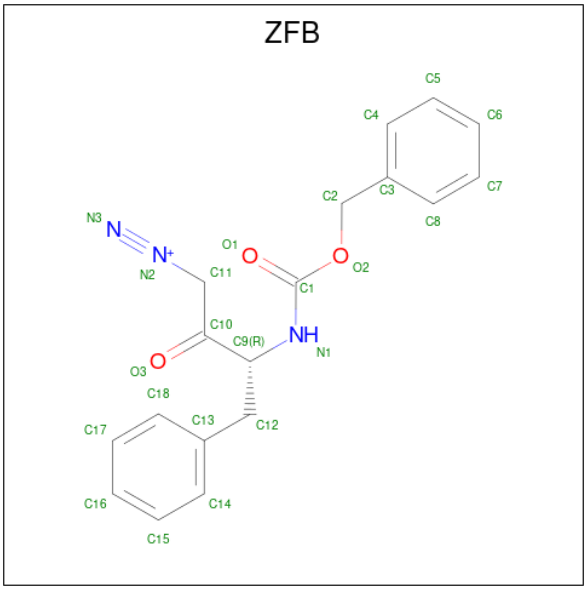
There are 3 unique types of molecules in this entry. The entry contains 11052 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 pyrogenic exotoxin B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	339	2603	1644	450	502	7	0	0	0
1	B	339	2603	1644	450	502	7	0	0	0
1	C	339	2603	1644	450	502	7	0	0	0
1	D	339	2603	1644	450	502	7	0	0	0

- Molecule 2 is (3R)-3-{[(BENZYLOXY)CARBONYL]AMINO}-2-OXO-4-PHENYLBUTANE-1-DIAZONIUM (three-letter code: ZFB) (formula: $C_{18}H_{18}N_3O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	22	18	1	3	0	0
2	B	1	22	18	1	3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	C	1	22	18	1	3	0	0
			Total	C	N	O		
2	D	1	22	18	1	3	0	0

- Molecule 3 is water.

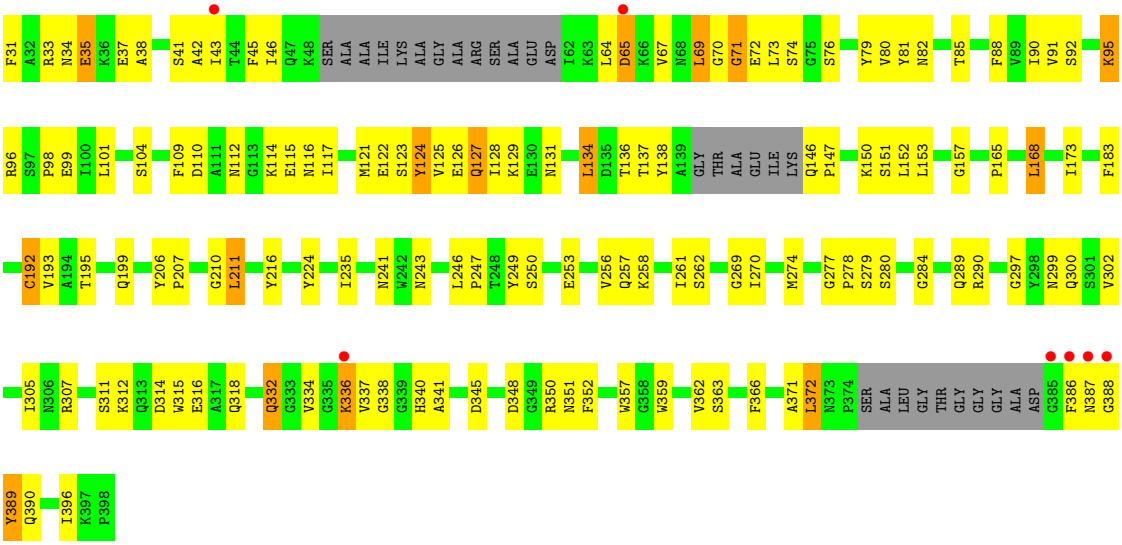
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	156	156	156	0	0
			Total	O		
3	B	128	128	128	0	0
			Total	O		
3	C	124	124	124	0	0
			Total	O		
3	D	144	144	144	0	0

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.

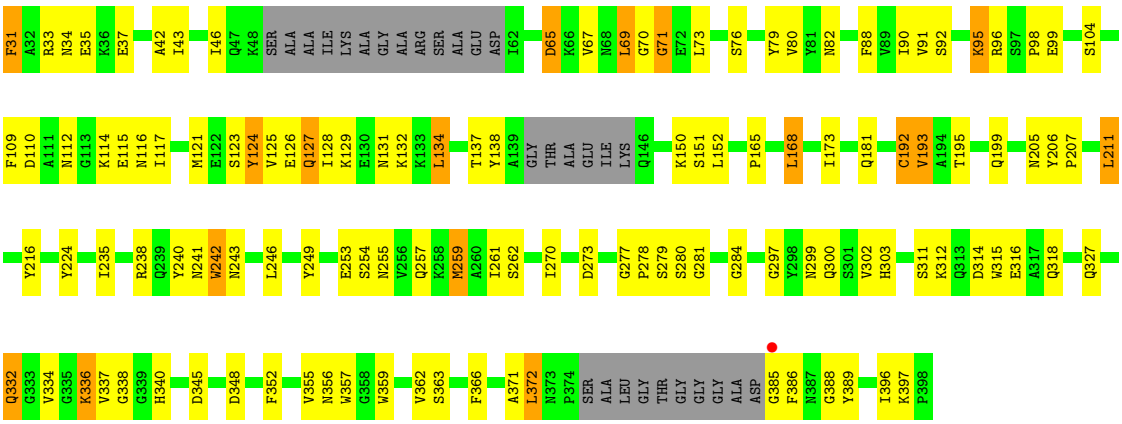
• Molecule 1: pyrogenic exotoxin B

Chain A: 2% 55% 33% 8%



• Molecule 1: pyrogenic exotoxin B

Chain B: 59% 29% 5% 8%



• Molecule 1: pyrogenic exotoxin B

Chain C: 60% 29% • 8%

F31 A32 R33 N34 E35 A42 I43 I46 Q47 K48 SER ALA ALA ILE LYS ALA GLY ALA ARG SER ALA GLU ASP I62 K63 L64 D65 K66 V67 N68 L69 G70 G71 E72 L73 S76 Y79 V80 Y81 N82 F88 V89 I90 V91 S92 R96 S97 P98 E99 I100 L101 S104

F109 D110 A111 N112 G113 K114 E115 N116 M121 E122 S123 Y124 V125 E126 Q127 I128 K129 E130 N131 K132 K133 L134 T137 Y138 A139 GLY THR ALA GLU ILE LYS Q146 K150 S151 L152 L153 G157 P165 L168 I173 P178 Q181 S182 F183 C192 V193 A194 T195 Q199

Y206 P207 L211 Y216 Y224 P228 L231 N241 W242 N243 L246 P247 E253 S254 N255 V256 Q257 K258 M259 A260 I261 S262 I270 G277 P278 S279 S280 G284 S285 G297 Y298 N299 Q300 S301 V302 R307 K312 W315 E316 A317 Q318 Q325 N326

Q327 Q332 K336 V337 G338 G339 H340 D345 D348 F352 W359 V362 S363 F366 D370 A371 L372 N373 P374 SER ALA LEU GLY THR GLY GLY GLY ALA ASP G385 F386 N387 G388 Y389 I396 K397 P398

• Molecule 1: pyrogenic exotoxin B

Chain D: 2% 54% 34% • 8%

F31 A32 R33 N34 E35 K36 E37 A38 K39 D40 S41 A42 I43 I46 Q47 K48 SER ALA ALA ILE LYS ALA GLY ALA ARG SER ALA GLU ASP I62 K63 L64 D65 K66 V67 N68 L69 G70 G71 E72 L73 S76 N77 M78 Y79 V80 Y81 N82 T85 F88 V89 I90 K95 R96 S97

P98 E99 I100 L101 S104 F109 D110 A111 N112 G113 K114 I117 M121 E122 S123 Y124 V125 E126 Q127 I128 K129 E130 N131 L134 D135 T136 T137 Y138 A139 GLY THR ALA GLU ILE LYS Q146 K150 S151 L152 L153 G157 I158 H159 P165 Y166 N167 L168 I173 F183

Q186 A189 C192 V193 A194 T195 Q199 N205 Y206 P207 N208 K209 G210 L211 Y216 Y224 K229 N230 L231 I235 R238 Q239 Y240 N241 W242 N243 L246 Y249 E253 S254 Q257 K258 M259 A260 I261 S262 G269 I270 M274 G277 P278 S279 S280

G284 S285 Q289 R290 N299 Q300 S301 V302 I305 N306 R307 S311 K312 Q313 D314 W315 E316 K321 Q327 Q332 G333 V334 G335 K336 V337 H340 A341 D345 D348 G349 R350 N351 F352 W359 V362 S363 F366 A371 L372 N373 P374 SER ALA LEU GLY THR

GLY GLY GLY ALA ASP G385 F386 N387 G388 Y389 I396 K397 P398

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	95.77Å 119.50Å 144.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 3.00 47.82 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (45.00-3.00) 88.5 (47.82-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	3.30 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.288 0.257 , 0.321	Depositor DCC
R_{free} test set	2070 reflections (6.95%)	wwPDB-VP
Wilson B-factor (Å^2)	25.4	Xtriage
Anisotropy	0.882	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 40.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	11052	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.75 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.1847e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZFB

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.85	1/2662 (0.0%)	0.83	1/3598 (0.0%)
1	B	0.75	1/2662 (0.0%)	0.82	1/3598 (0.0%)
1	C	0.77	1/2662 (0.0%)	0.82	2/3598 (0.1%)
1	D	0.81	1/2662 (0.0%)	0.82	1/3598 (0.0%)
All	All	0.80	4/10648 (0.0%)	0.82	5/14392 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	192	CYS	CB-SG	-13.56	1.59	1.82
1	C	192	CYS	CB-SG	-11.49	1.62	1.82
1	D	192	CYS	CB-SG	-10.34	1.64	1.82
1	B	192	CYS	CB-SG	-9.49	1.66	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	192	CYS	CA-CB-SG	8.15	128.67	114.00
1	D	192	CYS	CA-CB-SG	7.83	128.10	114.00
1	C	192	CYS	CA-CB-SG	7.18	126.92	114.00
1	A	192	CYS	CA-CB-SG	7.14	126.86	114.00
1	C	192	CYS	CB-CA-C	-5.19	100.02	110.40

There are no chirality outliers.

There are no planarity outliers.

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	2603	0	2472	120	0
1	B	2603	0	2472	105	0
1	C	2603	0	2472	101	0
1	D	2603	0	2472	126	0
2	A	22	0	13	18	0
2	B	22	0	13	16	0
2	C	22	0	13	17	0
2	D	22	0	12	17	0
3	A	156	0	0	3	0
3	B	128	0	0	4	0
3	C	124	0	0	4	0
3	D	144	0	0	9	0
All	All	11052	0	9939	464	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 23.

The worst 5 of 464 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:280:SER:H	2:B:450:ZFB:H15	1.03	1.14
1:C:280:SER:H	2:C:450:ZFB:H15	0.98	1.13
1:D:280:SER:H	2:D:450:ZFB:H15	1.04	1.12
1:A:280:SER:H	2:A:450:ZFB:H15	1.00	1.06
1:B:246:LEU:HD11	1:B:257:GLN:HG2	1.46	0.98

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	331/368 (90%)	306 (92%)	20 (6%)	5 (2%)	10	42
1	B	331/368 (90%)	301 (91%)	24 (7%)	6 (2%)	8	37
1	C	331/368 (90%)	300 (91%)	25 (8%)	6 (2%)	8	37
1	D	331/368 (90%)	300 (91%)	25 (8%)	6 (2%)	8	37
All	All	1324/1472 (90%)	1207 (91%)	94 (7%)	23 (2%)	9	39

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	GLU
1	A	337	VAL
1	B	35	GLU
1	B	337	VAL
1	C	35	GLU

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	272/297 (92%)	259 (95%)	13 (5%)	25	62
1	B	272/297 (92%)	259 (95%)	13 (5%)	25	62
1	C	272/297 (92%)	260 (96%)	12 (4%)	28	65
1	D	272/297 (92%)	260 (96%)	12 (4%)	28	65
All	All	1088/1188 (92%)	1038 (95%)	50 (5%)	27	64

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	69	LEU
1	C	332	GLN
1	D	372	LEU

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Mol	Chain	Res	Type
1	C	124	TYR
1	C	168	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	318	GLN
1	D	208	ASN
1	C	332	GLN
1	D	243	ASN
1	B	243	ASN

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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
2	ZFB	A	450	1	23,23,25	5.08	16 (69%)	25,29,31	3.13	8 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ZFB	B	450	1	23,23,25	5.08	18 (78%)	25,29,31	3.14	9 (36%)
2	ZFB	D	450	1	23,23,25	5.07	17 (73%)	25,29,31	3.08	7 (28%)
2	ZFB	C	450	1	23,23,25	5.25	19 (82%)	25,29,31	3.14	8 (32%)

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	ZFB	A	450	1	-	11/17/17/20	0/2/2/2
2	ZFB	B	450	1	-	13/17/17/20	0/2/2/2
2	ZFB	D	450	1	-	12/17/17/20	0/2/2/2
2	ZFB	C	450	1	-	9/17/17/20	0/2/2/2

The worst 5 of 70 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	450	ZFB	O2-C1	11.59	1.57	1.35
2	C	450	ZFB	O2-C1	11.53	1.57	1.35
2	A	450	ZFB	C12-C9	-11.44	1.25	1.54
2	C	450	ZFB	C12-C9	-11.33	1.25	1.54
2	D	450	ZFB	O2-C1	10.92	1.56	1.35

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	450	ZFB	O2-C2-C3	8.09	128.83	109.39
2	C	450	ZFB	O2-C2-C3	8.01	128.65	109.39
2	D	450	ZFB	O2-C2-C3	7.95	128.50	109.39
2	A	450	ZFB	O2-C2-C3	7.88	128.32	109.39
2	A	450	ZFB	C2-O2-C1	7.69	133.09	115.93

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	450	ZFB	O1-C1-N1-C9
2	A	450	ZFB	O2-C1-N1-C9
2	A	450	ZFB	C10-C9-N1-C1

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Mol	Chain	Res	Type	Atoms
2	A	450	ZFB	N1-C1-O2-C2
2	A	450	ZFB	O1-C1-O2-C2

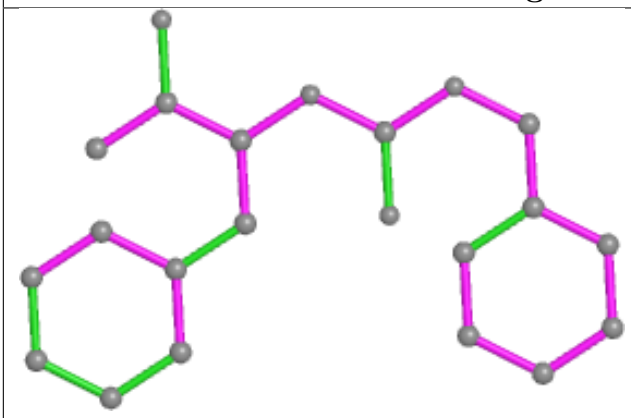
There are no ring outliers.

4 monomers are involved in 68 short contacts:

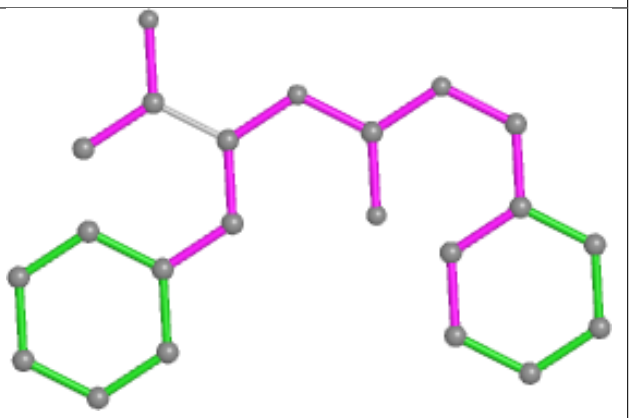
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	450	ZFB	18	0
2	B	450	ZFB	16	0
2	D	450	ZFB	17	0
2	C	450	ZFB	17	0

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.

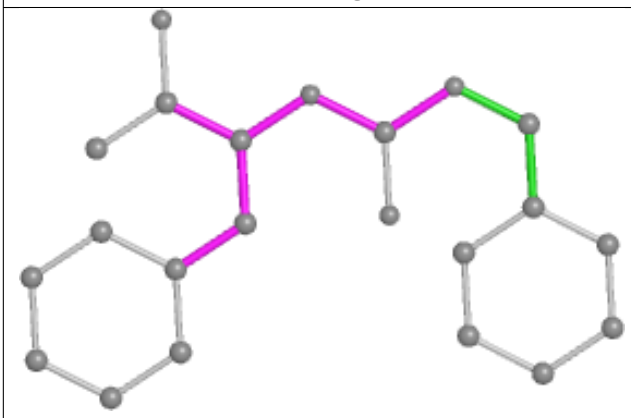
Ligand ZFB A 450



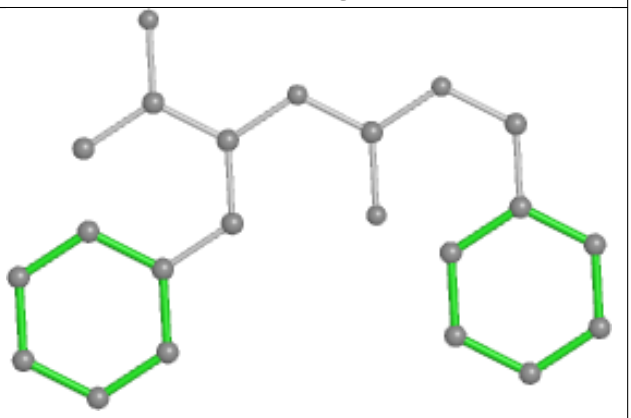
Bond lengths



Bond angles

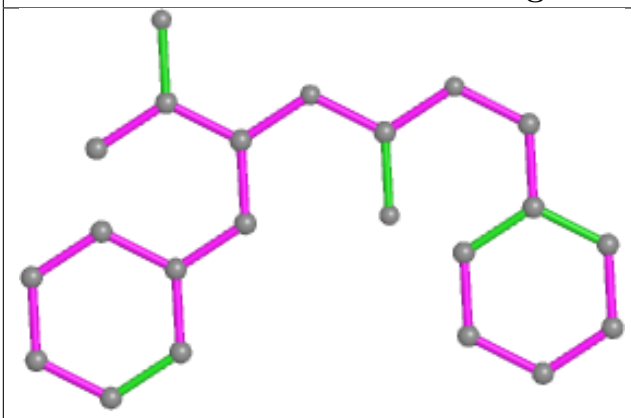


Torsions

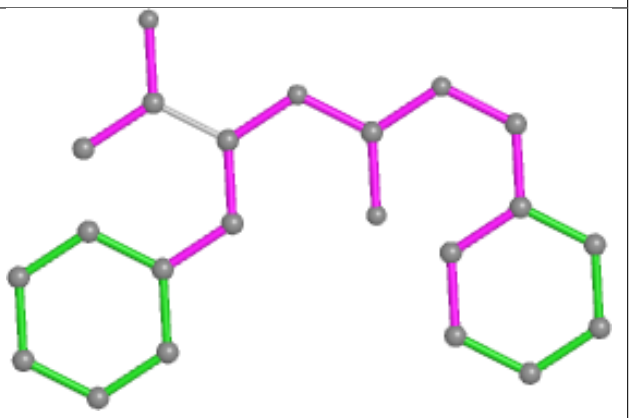


Rings

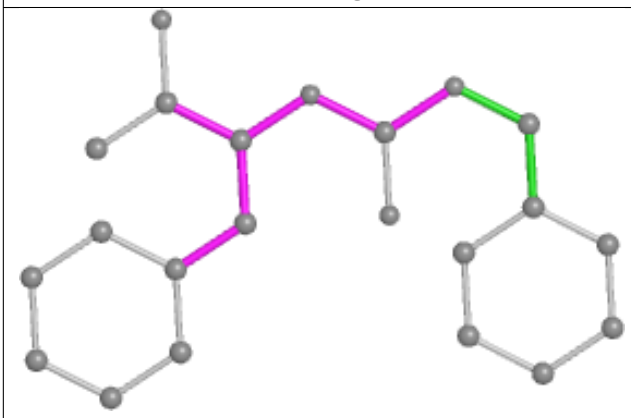
Ligand ZFB B 450



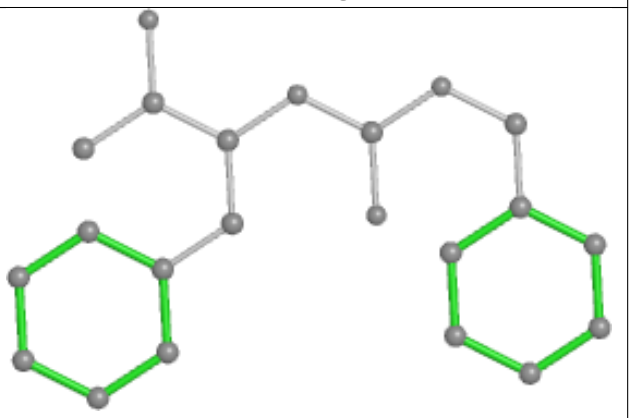
Bond lengths



Bond angles

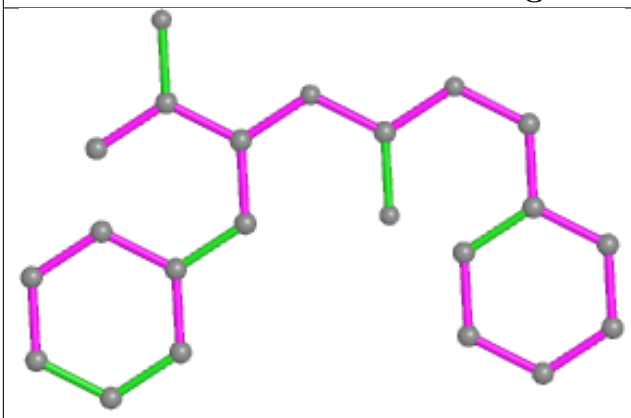


Torsions

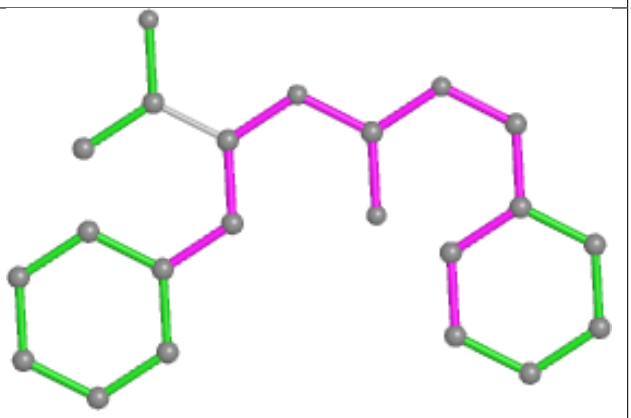


Rings

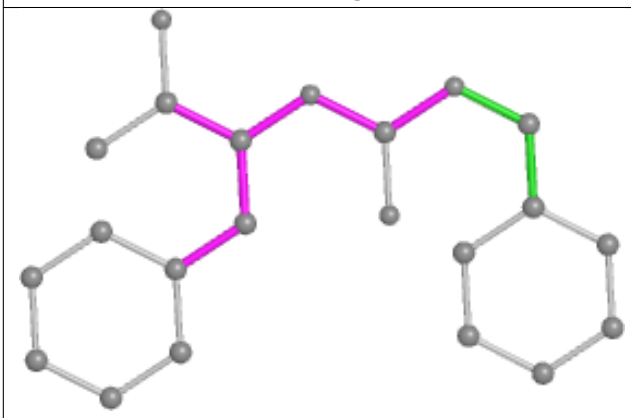
Ligand ZFB D 450



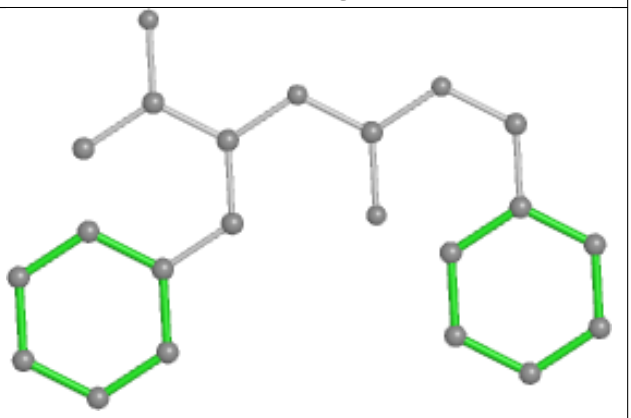
Bond lengths



Bond angles

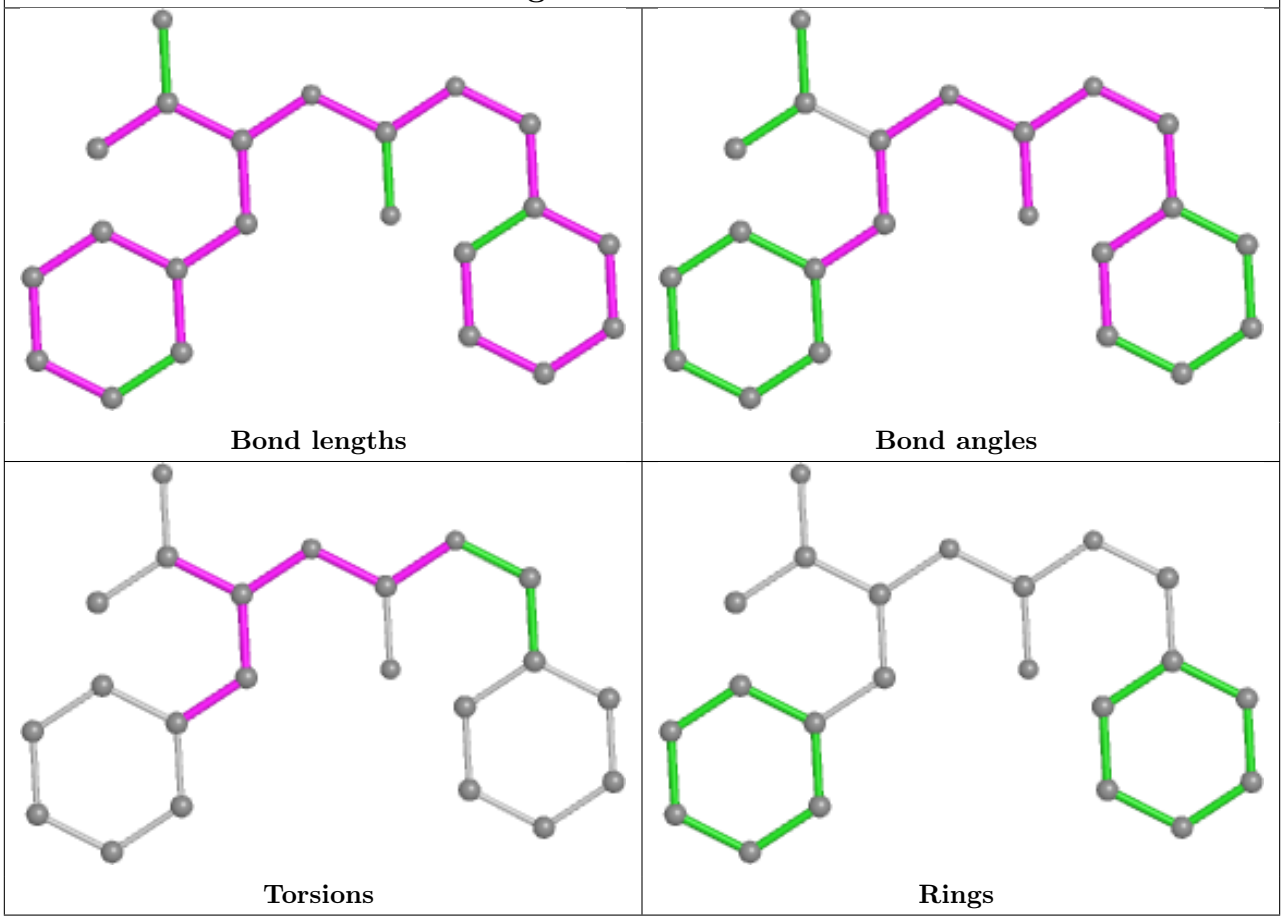


Torsions



Rings

Ligand ZFB C 450



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	339/368 (92%)	-0.15	7 (2%)	63	34	9, 17, 25, 29	0
1	B	339/368 (92%)	-0.22	1 (0%)	94	84	9, 17, 25, 29	0
1	C	339/368 (92%)	-0.25	1 (0%)	94	84	9, 17, 25, 29	0
1	D	339/368 (92%)	-0.17	6 (1%)	68	40	9, 17, 25, 29	0
All	All	1356/1472 (92%)	-0.20	15 (1%)	80	56	9, 17, 25, 29	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	387	ASN	6.0
1	A	387	ASN	5.3
1	D	385	GLY	4.8
1	A	386	PHE	4.4
1	A	385	GLY	4.2

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

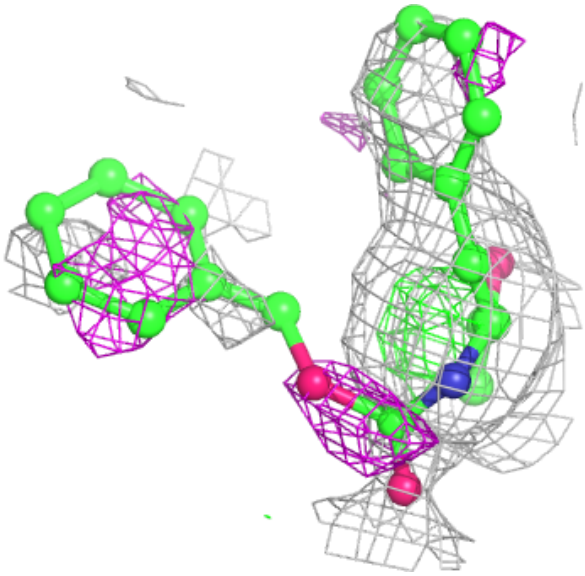
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

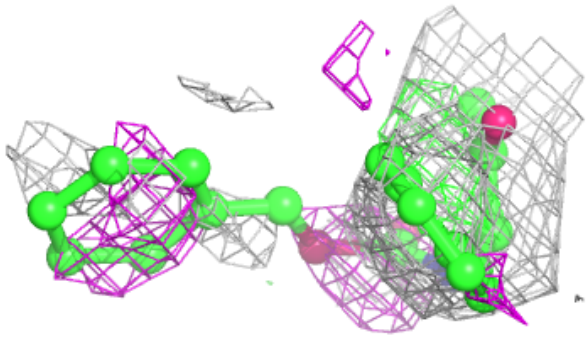
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZFB	A	450	22/24	0.75	0.50	23,28,31,31	0
2	ZFB	C	450	22/24	0.75	0.43	23,28,31,31	0
2	ZFB	B	450	22/24	0.76	0.42	23,28,31,31	0
2	ZFB	D	450	22/24	0.82	0.40	23,28,31,31	0

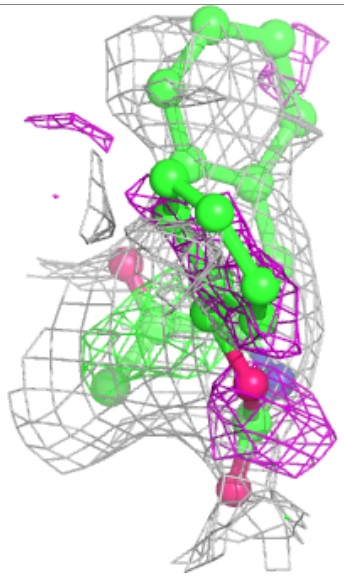
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ZFB A 450:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

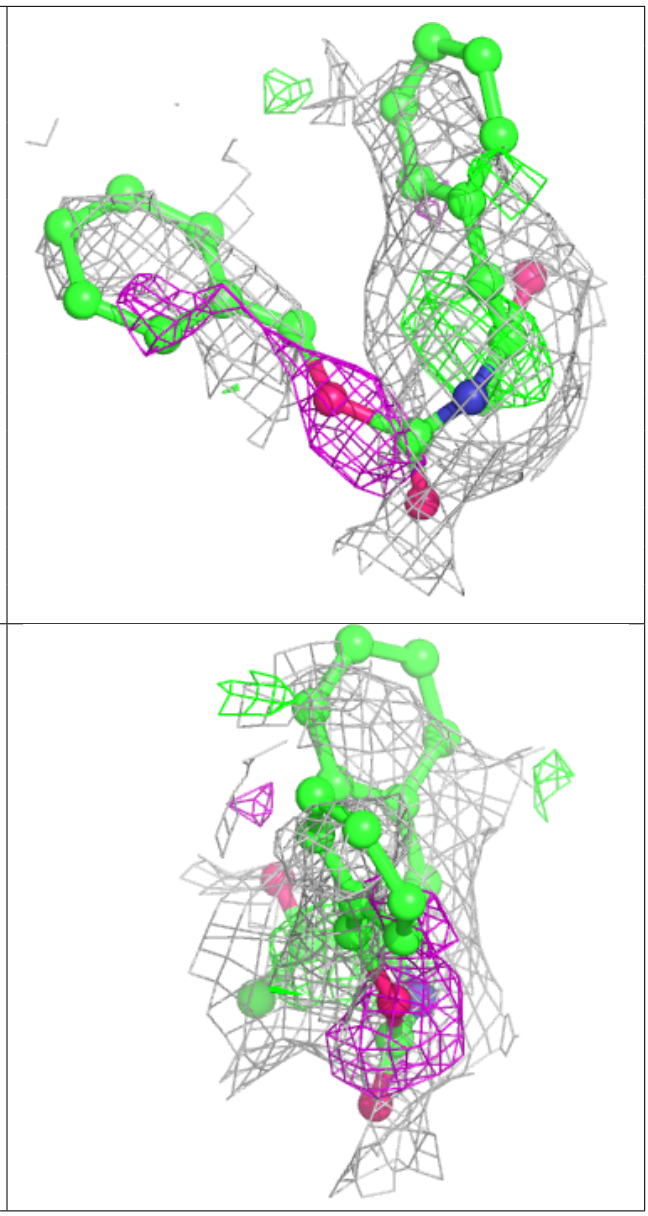






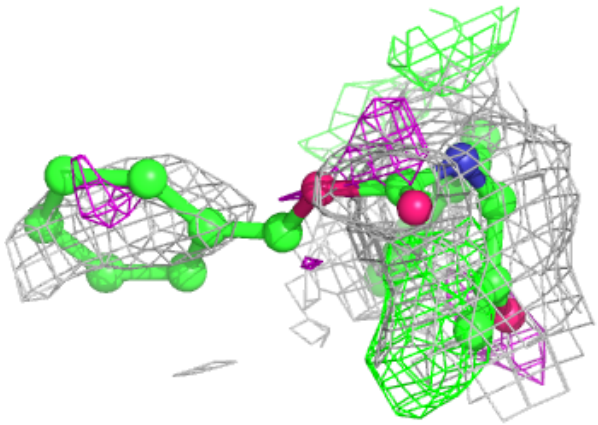
Electron density around ZFB C 450:

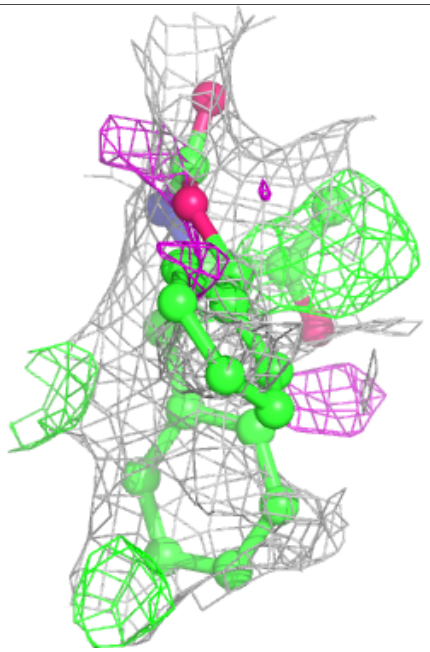
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZFB B 450:

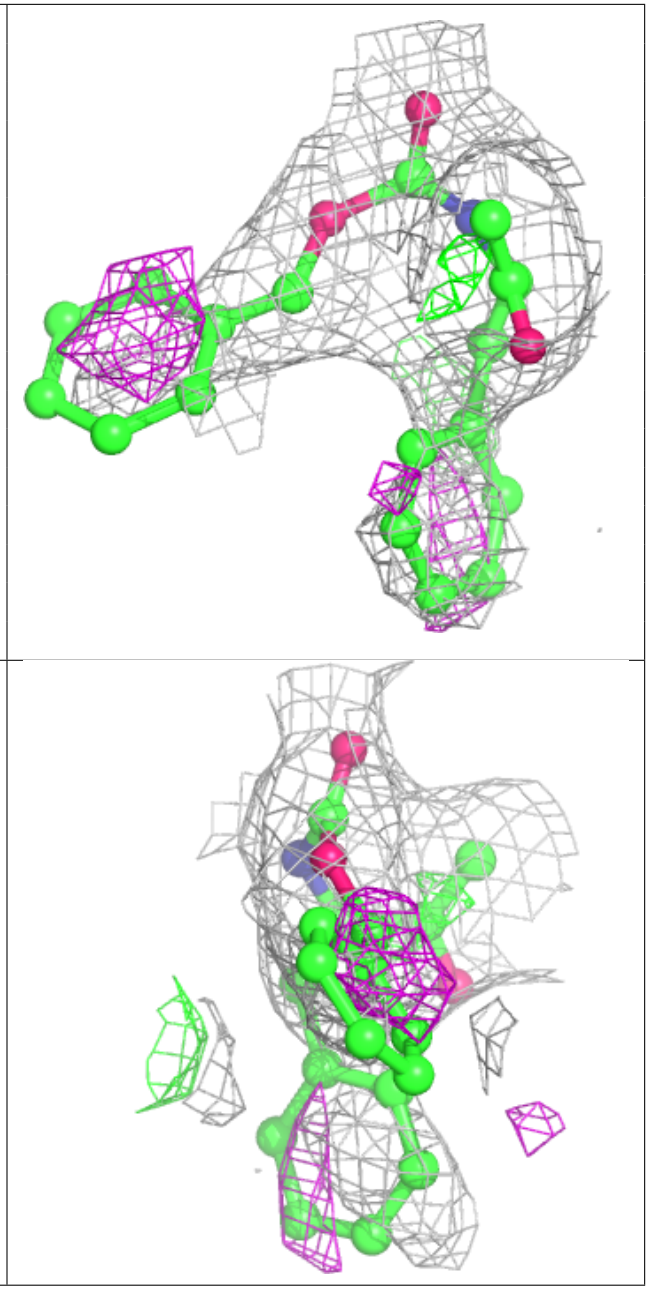
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around ZFB D 450:

$2mF_o$-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.