



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 12:12 am BST

PDB ID : 6EPH  
Title : Structure of the epsilon\_1 / zeta\_1 antitoxin toxin system from *Neisseria gonorrhoeae* in complex with UNAM.  
Authors : Rocker, A.; Meinhart, A.  
Deposited on : 2017-10-11  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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 : 2.11  
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) : 2.11

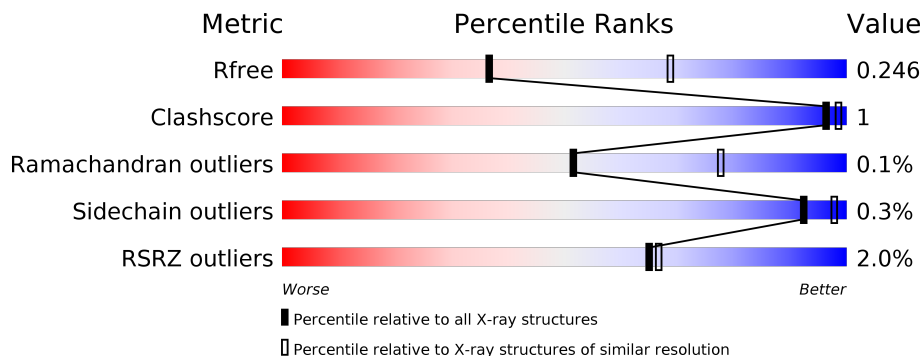
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\geq 3$ , 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	61	
1	C	61	
1	E	61	
1	G	61	
2	B	401	
2	D	401	

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Mol	Chain	Length	Quality of chain
2	F	401	<p>%</p> <p>96%</p>
2	H	401	<p>%</p> <p>95%</p>

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
5	FLC	F	504	-	-	-	X

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 14405 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.

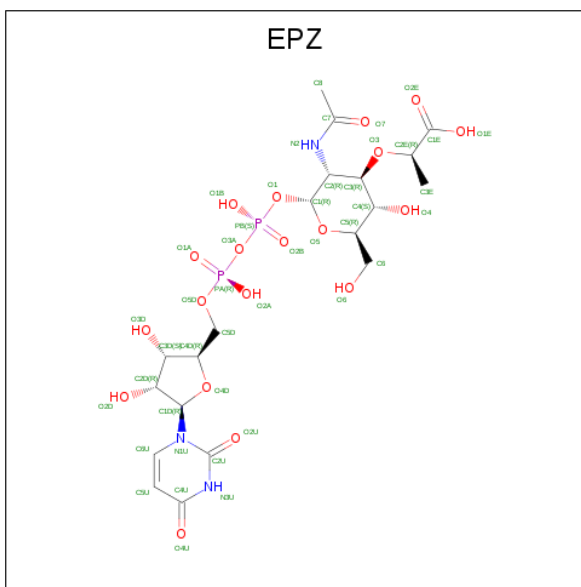
- Molecule 1 is a protein called Epsilon\_1 antitoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	53	Total 433	C 270	N 81	O 78	S 4	0	0	0
1	C	53	Total 433	C 270	N 82	O 77	S 4	0	0	0
1	E	52	Total 424	C 265	N 80	O 75	S 4	0	0	0
1	G	53	Total 433	C 270	N 82	O 77	S 4	0	0	0

- Molecule 2 is a protein called Zeta\_1 toxin.

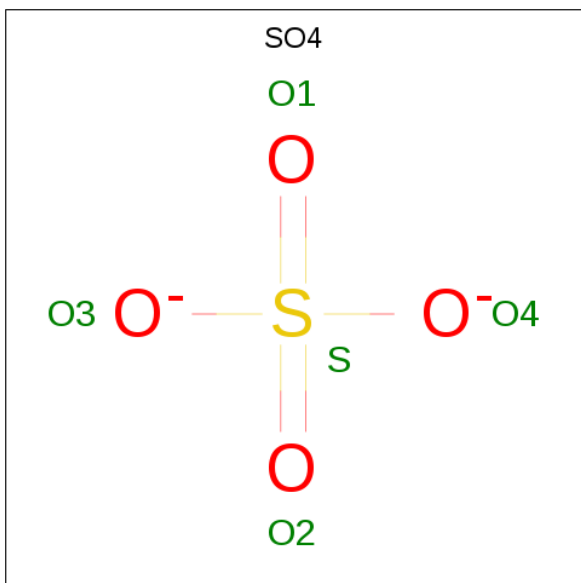
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	394	Total 3079	C 1917	N 539	O 612	S 11	0	0	0
2	D	394	Total 3079	C 1917	N 539	O 612	S 11	0	0	0
2	F	394	Total 3079	C 1917	N 539	O 612	S 11	0	0	0
2	H	394	Total 3079	C 1917	N 539	O 612	S 11	0	0	0

- Molecule 3 is (2R)-2-(((2R,3R,4R,5S,6R)-3-(acetylamino)-2-(((S)-(((R)-((2R,3S,4R,5R)-5-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-3,4-dihydroxytetrahydrofuran-2-yl)methoxy)(hydroxy)phosphoryl]oxy)(hydroxy)phosphoryl]oxy)-5-hydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-4-yl]oxy)propanoic acid (three-letter code: EPZ) (formula: C<sub>20</sub>H<sub>31</sub>N<sub>3</sub>O<sub>19</sub>P<sub>2</sub>).



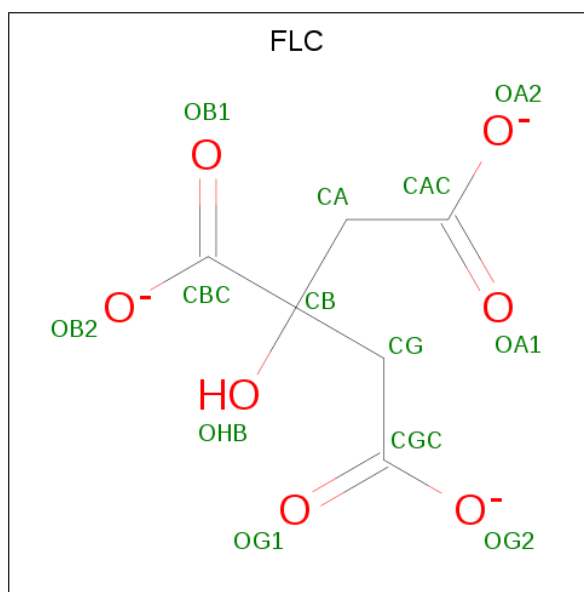
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
3	B	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	D	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	F	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	H	1	Total	C	N	O	P	0	0
			44	20	3	19	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0

- Molecule 5 is CITRATE ANION (three-letter code: FLC) (formula:  $C_6H_5O_7^-$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			13	6	7		
5	F	1	Total	C	O	0	0
			13	6	7		

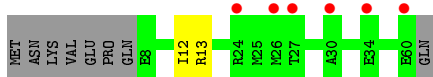
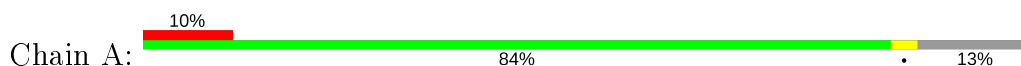
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		
6	B	23	Total	O	0	0
			23	23		
6	C	3	Total	O	0	0
			3	3		
6	D	23	Total	O	0	0
			23	23		
6	E	2	Total	O	0	0
			2	2		
6	F	28	Total	O	0	0
			28	28		
6	G	3	Total	O	0	0
			3	3		
6	H	21	Total	O	0	0
			21	21		

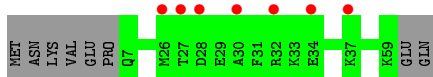
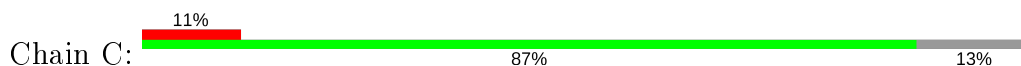
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

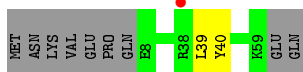
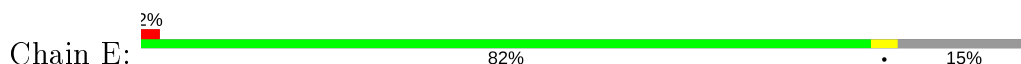
- Molecule 1: Epsilon\_1 antitoxin



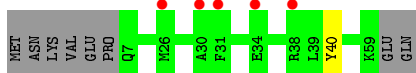
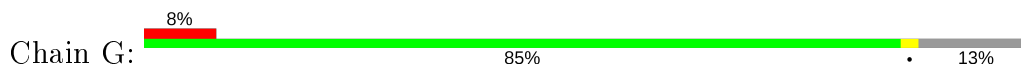
- Molecule 1: Epsilon\_1 antitoxin



- Molecule 1: Epsilon\_1 antitoxin



- Molecule 1: Epsilon\_1 antitoxin



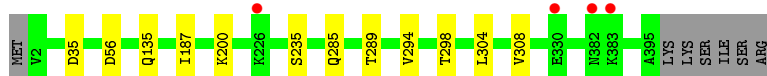
- Molecule 2: Zeta\_1 toxin



- Molecule 2: Zeta\_1 toxin



Chain D:  95%



• Molecule 2: Zeta\_1 toxin

Chain F:  96%



• Molecule 2: Zeta\_1 toxin

Chain H:  95%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.29Å 148.18Å 124.40Å 90.00° 93.88° 90.00°	Depositor
Resolution (Å)	49.00 – 2.70 49.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.00-2.70) 99.4 (49.00-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.220 , 0.245 0.224 , 0.246	Depositor DCC
$R_{free}$ test set	4064 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.5	Xtrriage
Anisotropy	0.499	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 34.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14405	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.32 % 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 2.0737e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FLC, EPZ, SO4

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	0.38	0/438	0.59	0/583
1	C	0.38	0/438	0.58	0/583
1	E	0.37	0/429	0.58	0/571
1	G	0.38	0/438	0.59	0/583
2	B	0.36	0/3117	0.56	0/4186
2	D	0.36	0/3117	0.56	0/4186
2	F	0.36	0/3117	0.56	0/4186
2	H	0.36	0/3117	0.56	0/4186
All	All	0.36	0/14211	0.56	0/19064

There are no bond length outliers.

There are no bond angle outliers.

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	433	0	449	2	0
1	C	433	0	451	0	0
1	E	424	0	443	2	0
1	G	433	0	451	1	0
2	B	3079	0	3080	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3079	0	3080	7	0
2	F	3079	0	3080	7	0
2	H	3079	0	3080	9	0
3	B	44	0	28	2	0
3	D	44	0	28	2	0
3	F	44	0	28	2	0
3	H	44	0	28	2	0
4	B	20	0	0	0	0
4	D	10	0	0	0	0
4	F	10	0	0	0	0
4	H	20	0	0	0	0
5	D	13	0	5	0	0
5	F	13	0	5	0	0
6	A	1	0	0	0	0
6	B	23	0	0	0	0
6	C	3	0	0	0	0
6	D	23	0	0	0	0
6	E	2	0	0	0	0
6	F	28	0	0	0	0
6	G	3	0	0	0	0
6	H	21	0	0	0	0
All	All	14405	0	14236	29	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 1.

All (29) 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)
2:H:135:GLN:HG2	3:H:501:EPZ:H8B	1.79	0.63
2:B:135:GLN:HG2	3:B:501:EPZ:H8B	1.83	0.59
2:B:197:ASP:HA	2:D:304:LEU:HD21	1.84	0.59
2:D:135:GLN:HG2	3:D:501:EPZ:H8B	1.86	0.57
2:F:135:GLN:HG2	3:F:501:EPZ:H8B	1.89	0.55
2:B:285:GLN:HG2	2:B:298:THR:HG22	1.91	0.52
2:F:304:LEU:HD21	2:H:197:ASP:HA	1.93	0.50
1:G:40:TYR:CD2	2:H:175:ARG:HD2	2.47	0.50
2:D:187:ILE:HD11	3:D:501:EPZ:C7	2.43	0.49
2:B:304:LEU:HD22	2:D:200:LYS:HD3	1.95	0.48
2:F:187:ILE:HD11	3:F:501:EPZ:C7	2.44	0.48
2:H:285:GLN:HG2	2:H:298:THR:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:321:TYR:CG	2:B:340:ILE:HD13	2.51	0.46
2:B:298:THR:HG23	2:B:308:VAL:HG21	1.97	0.46
1:E:40:TYR:CD1	2:F:175:ARG:HD2	2.52	0.45
2:H:93:VAL:HG11	2:H:130:LEU:HD13	1.99	0.44
2:H:187:ILE:HD11	3:H:501:EPZ:C7	2.47	0.44
2:H:298:THR:HG23	2:H:308:VAL:HG21	1.99	0.44
2:F:298:THR:HG23	2:F:308:VAL:HG21	1.98	0.44
2:D:285:GLN:CG	2:D:298:THR:HG22	2.48	0.44
2:B:285:GLN:CG	2:B:298:THR:HG22	2.47	0.43
2:B:187:ILE:HD11	3:B:501:EPZ:H8A	1.99	0.43
2:D:298:THR:HG23	2:D:308:VAL:HG21	2.00	0.43
1:A:12:ILE:HD11	2:B:211:LYS:HG2	2.00	0.43
2:F:285:GLN:CG	2:F:298:THR:HG22	2.49	0.42
2:D:289:THR:HG22	2:D:294:VAL:HG12	2.01	0.42
2:H:90:PHE:CD2	2:H:130:LEU:HD21	2.55	0.41
1:A:13:ARG:HD2	2:H:125:GLN:HA	2.03	0.41
1:E:39:LEU:HD22	2:F:116:THR:HG22	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	51/61 (84%)	50 (98%)	1 (2%)	0	100	100
1	C	51/61 (84%)	50 (98%)	1 (2%)	0	100	100
1	E	50/61 (82%)	49 (98%)	1 (2%)	0	100	100
1	G	51/61 (84%)	50 (98%)	1 (2%)	0	100	100
2	B	392/401 (98%)	384 (98%)	8 (2%)	0	100	100
2	D	392/401 (98%)	386 (98%)	5 (1%)	1 (0%)	41	66
2	F	392/401 (98%)	382 (97%)	9 (2%)	1 (0%)	41	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	392/401 (98%)	385 (98%)	7 (2%)	0	100	100
All	All	1771/1848 (96%)	1736 (98%)	33 (2%)	2 (0%)	51	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	235	SER
2	F	235	SER

### 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	45/53 (85%)	45 (100%)	0	100	100
1	C	45/53 (85%)	45 (100%)	0	100	100
1	E	44/53 (83%)	44 (100%)	0	100	100
1	G	45/53 (85%)	45 (100%)	0	100	100
2	B	336/343 (98%)	335 (100%)	1 (0%)	92	98
2	D	336/343 (98%)	334 (99%)	2 (1%)	86	95
2	F	336/343 (98%)	336 (100%)	0	100	100
2	H	336/343 (98%)	334 (99%)	2 (1%)	86	95
All	All	1523/1584 (96%)	1518 (100%)	5 (0%)	92	98

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	35	ASP
2	D	35	ASP
2	D	56	ASP
2	H	56	ASP
2	H	208	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	265	ASN
2	F	43	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

18 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	SO4	F	502	-	4,4,4	0.36	0	6,6,6	0.09	0
4	SO4	B	504	-	4,4,4	0.33	0	6,6,6	0.14	0
4	SO4	B	502	-	4,4,4	0.31	0	6,6,6	0.12	0
3	EPZ	F	501	-	36,46,46	0.76	1 (2%)	46,69,69	1.03	4 (8%)
4	SO4	B	505	-	4,4,4	0.32	0	6,6,6	0.07	0
4	SO4	H	504	-	4,4,4	0.32	0	6,6,6	0.12	0
4	SO4	D	502	-	4,4,4	0.33	0	6,6,6	0.17	0
5	FLC	D	504	-	3,12,12	0.61	0	3,17,17	3.36	3 (100%)
4	SO4	H	503	-	4,4,4	0.31	0	6,6,6	0.11	0
4	SO4	F	503	-	4,4,4	0.30	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	H	502	-	4,4,4	0.32	0	6,6,6	0.09	0
4	SO4	D	503	-	4,4,4	0.34	0	6,6,6	0.19	0
5	FLC	F	504	-	3,12,12	0.96	0	3,17,17	2.28	1 (33%)
4	SO4	B	503	-	4,4,4	0.31	0	6,6,6	0.15	0
3	EPZ	H	501	-	36,46,46	0.76	1 (2%)	46,69,69	1.04	4 (8%)
3	EPZ	D	501	-	36,46,46	0.78	2 (5%)	46,69,69	1.03	3 (6%)
4	SO4	H	505	-	4,4,4	0.37	0	6,6,6	0.09	0
3	EPZ	B	501	-	36,46,46	0.77	1 (2%)	46,69,69	1.05	4 (8%)

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	EPZ	F	501	-	-	5/28/71/71	0/3/3/3
3	EPZ	B	501	-	-	6/28/71/71	0/3/3/3
5	FLC	D	504	-	-	5/6/16/16	-
5	FLC	F	504	-	-	4/6/16/16	-
3	EPZ	H	501	-	-	6/28/71/71	0/3/3/3
3	EPZ	D	501	-	-	5/28/71/71	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	EPZ	C4U-N3U	3.56	1.39	1.33
3	F	501	EPZ	C4U-N3U	3.51	1.39	1.33
3	D	501	EPZ	C4U-N3U	3.49	1.39	1.33
3	H	501	EPZ	C4U-N3U	3.47	1.39	1.33
3	D	501	EPZ	PB-O1	-2.10	1.55	1.60

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	EPZ	C5U-C4U-N3U	-4.07	114.35	123.31
3	D	501	EPZ	C5U-C4U-N3U	-4.06	114.38	123.31
3	F	501	EPZ	C5U-C4U-N3U	-4.06	114.39	123.31
3	H	501	EPZ	C5U-C4U-N3U	-4.04	114.42	123.31
5	D	504	FLC	CB-CA-CAC	-3.91	108.72	114.98
5	F	504	FLC	CG-CB-CA	3.54	118.79	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	504	FLC	CG-CB-CA	3.49	118.65	109.33
3	H	501	EPZ	C3E-C2E-C1E	-3.11	109.33	113.35
3	F	501	EPZ	C3E-C2E-C1E	-3.02	109.44	113.35
3	D	501	EPZ	C3E-C2E-C1E	-2.96	109.52	113.35
3	B	501	EPZ	O3A-PB-O1	2.96	108.44	102.48
3	B	501	EPZ	C3E-C2E-C1E	-2.91	109.58	113.35
3	H	501	EPZ	C2-N2-C7	2.62	129.56	123.18
3	F	501	EPZ	C2-N2-C7	2.55	129.39	123.18
3	D	501	EPZ	C2-N2-C7	2.55	129.38	123.18
3	B	501	EPZ	C2-N2-C7	2.52	129.30	123.18
5	D	504	FLC	CB-CG-CGC	2.51	119.00	114.98
3	H	501	EPZ	C1-C2-N2	2.27	114.91	111.00
3	F	501	EPZ	C1-C2-N2	2.24	114.85	111.00

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	501	EPZ	PB-O3A-PA-O5D
5	D	504	FLC	CAC-CA-CB-CG
5	D	504	FLC	CBC-CB-CG-CGC
5	F	504	FLC	CAC-CA-CB-CBC
5	F	504	FLC	CA-CB-CG-CGC
3	H	501	EPZ	O5-C5-C6-O6
3	D	501	EPZ	C4-C5-C6-O6
3	D	501	EPZ	O5-C5-C6-O6
3	B	501	EPZ	C8-C7-N2-C2
3	B	501	EPZ	O5-C5-C6-O6
3	F	501	EPZ	O7-C7-N2-C2
3	F	501	EPZ	C8-C7-N2-C2
3	D	501	EPZ	O7-C7-N2-C2
3	D	501	EPZ	C8-C7-N2-C2
3	H	501	EPZ	O7-C7-N2-C2
3	H	501	EPZ	C8-C7-N2-C2
3	B	501	EPZ	O7-C7-N2-C2
3	F	501	EPZ	C4-C5-C6-O6
3	B	501	EPZ	C4-C5-C6-O6
3	H	501	EPZ	C4-C5-C6-O6
3	F	501	EPZ	O5-C5-C6-O6
3	B	501	EPZ	PB-O3A-PA-O1A
5	D	504	FLC	CAC-CA-CB-OHB
3	D	501	EPZ	PB-O3A-PA-O5D

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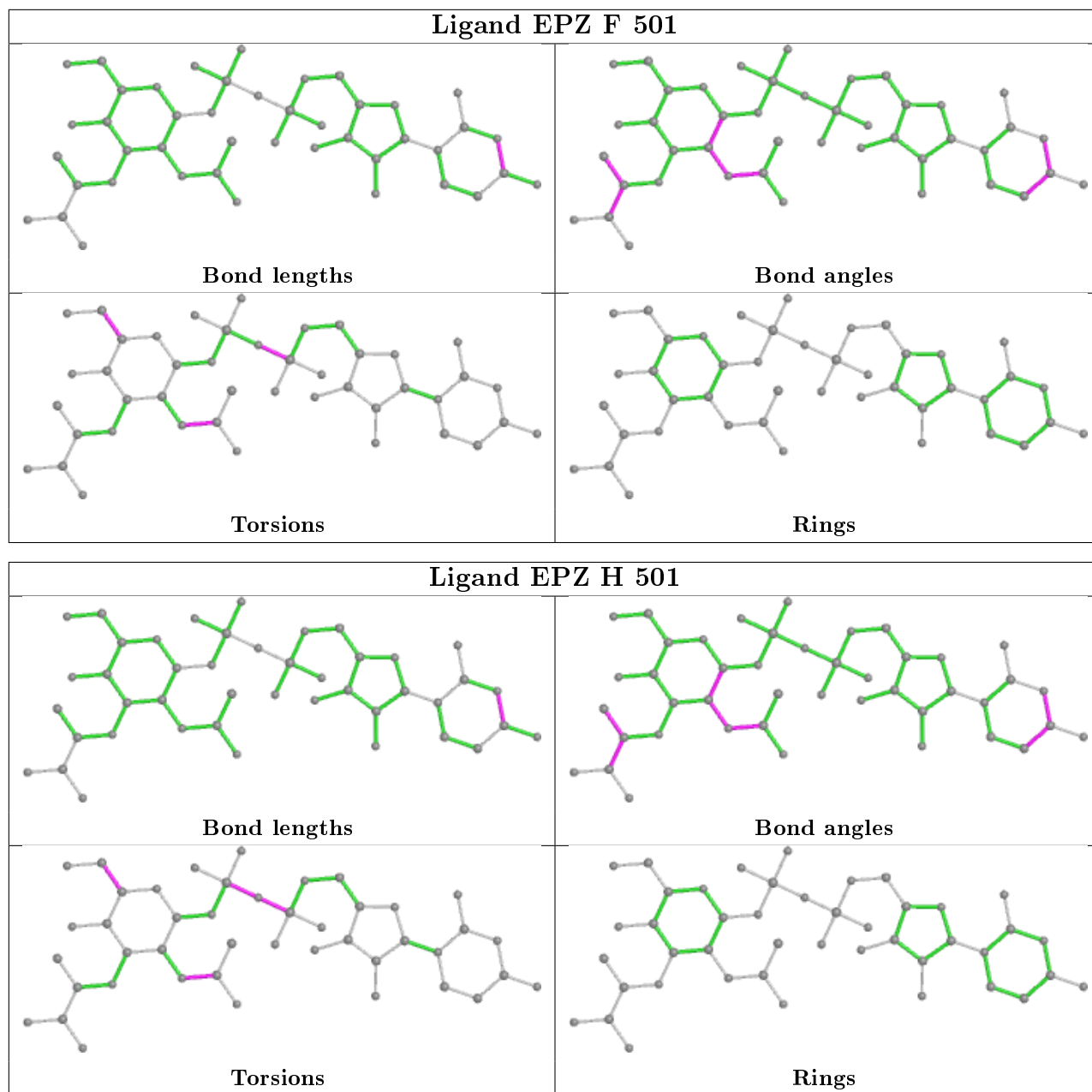
Mol	Chain	Res	Type	Atoms
3	H	501	EPZ	PB-O3A-PA-O5D
3	B	501	EPZ	C1-O1-PB-O3A
5	D	504	FLC	CAC-CA-CB-CBC
5	F	504	FLC	CBC-CB-CG-CGC
5	F	504	FLC	OHB-CB-CG-CGC
5	D	504	FLC	CA-CB-CG-CGC
3	H	501	EPZ	PA-O3A-PB-O1B

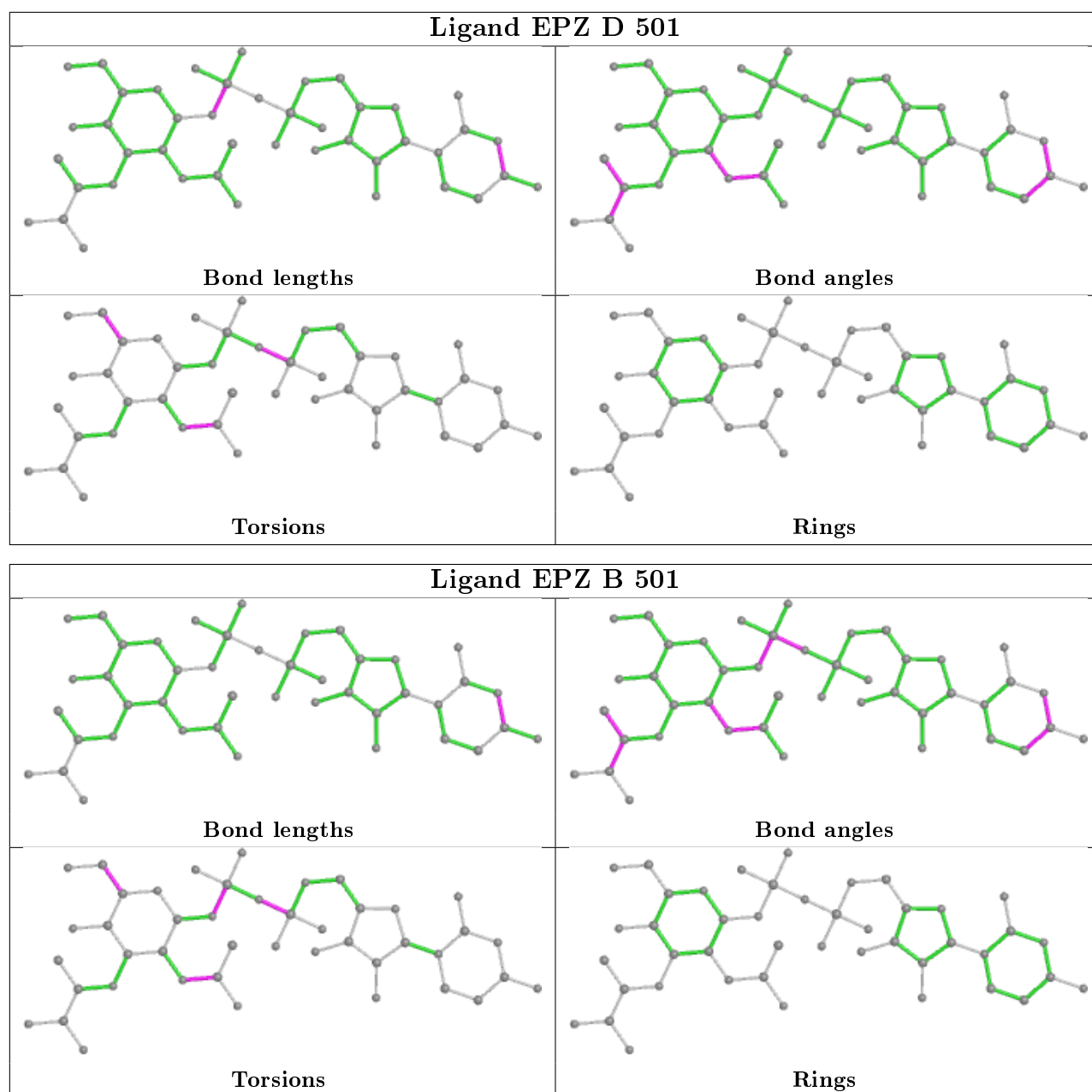
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	501	EPZ	2	0
3	H	501	EPZ	2	0
3	D	501	EPZ	2	0
3	B	501	EPZ	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.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	53/61 (86%)	0.49	6 (11%) 5 4	56, 81, 117, 124	0
1	C	53/61 (86%)	0.62	7 (13%) 3 2	51, 81, 130, 136	0
1	E	52/61 (85%)	0.42	1 (1%) 66 69	51, 83, 105, 119	0
1	G	53/61 (86%)	0.52	5 (9%) 8 6	58, 83, 126, 127	0
2	B	394/401 (98%)	0.11	3 (0%) 86 87	41, 61, 90, 130	0
2	D	394/401 (98%)	0.15	4 (1%) 82 83	42, 62, 91, 120	0
2	F	394/401 (98%)	0.12	3 (0%) 86 87	43, 62, 93, 111	0
2	H	394/401 (98%)	0.08	6 (1%) 73 76	38, 61, 88, 128	0
All	All	1787/1848 (96%)	0.16	35 (1%) 65 67	38, 63, 98, 136	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	30	ALA	4.0
1	C	34	GLU	3.6
1	G	30	ALA	3.6
1	C	27	THR	3.6
2	H	383	LYS	3.4
1	C	37	LYS	3.4
1	G	31	PHE	3.1
2	D	226	LYS	3.0
2	D	383	LYS	2.9
1	C	30	ALA	2.8
1	C	28	ASP	2.8
1	C	32	ARG	2.7
2	F	226	LYS	2.7
2	H	15	ASN	2.7
2	B	15	ASN	2.6
1	A	34	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	26	MET	2.5
1	G	26	MET	2.5
2	F	123	MET	2.5
2	B	383	LYS	2.5
1	E	38	ARG	2.4
2	B	43	GLN	2.3
2	H	226	LYS	2.3
2	H	44	HIS	2.2
1	G	34	GLU	2.2
2	D	330	GLU	2.2
1	A	26	MET	2.2
2	H	225	ASP	2.2
1	A	60	GLU	2.1
1	A	27	THR	2.1
2	D	382	ASN	2.1
2	F	382	ASN	2.1
2	H	10	LEU	2.1
1	A	24	ARG	2.0
1	G	38	ARG	2.0

## 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 carbohydrates 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, 95<sup>th</sup> 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.

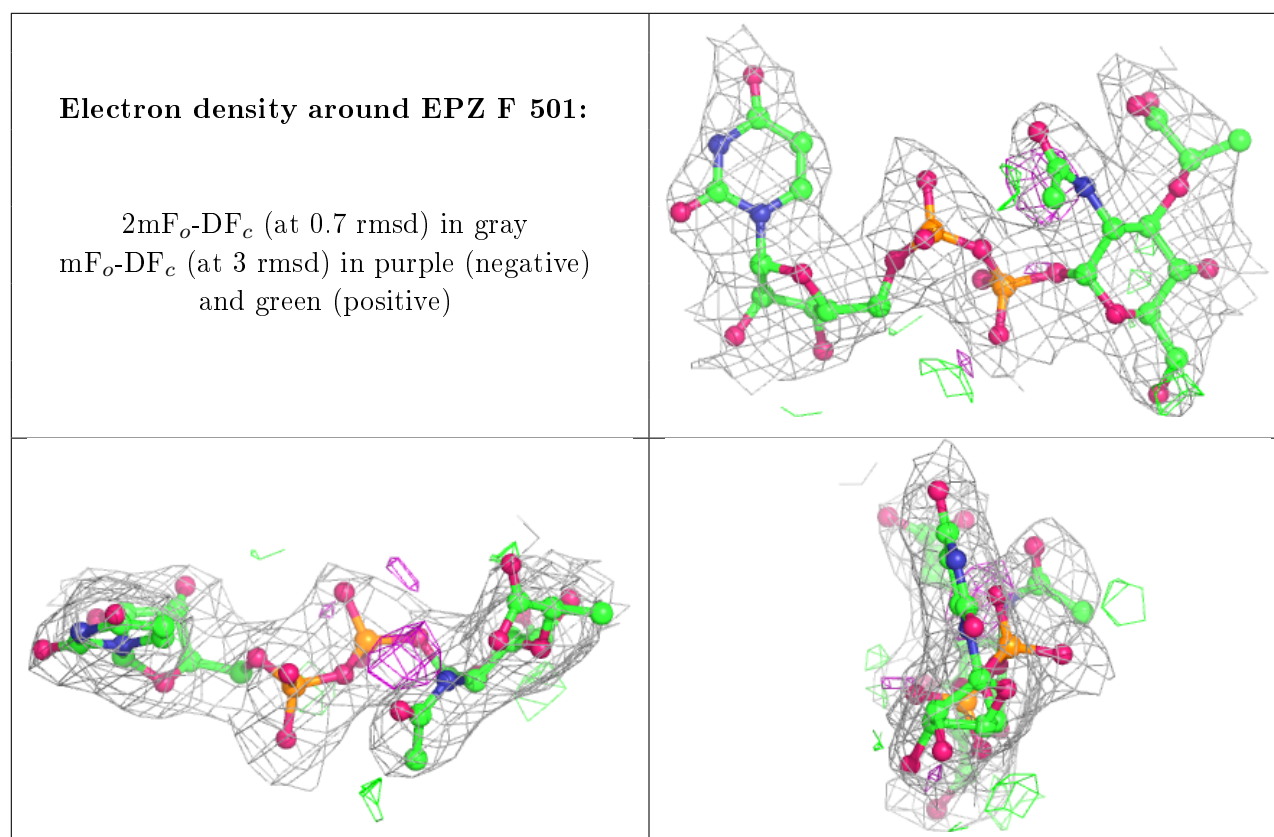
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	FLC	F	504	13/13	0.71	0.45	101,112,119,120	0
5	FLC	D	504	13/13	0.77	0.38	102,107,115,121	0
4	SO4	H	504	5/5	0.93	0.23	89,91,92,92	0
4	SO4	H	505	5/5	0.93	0.16	88,88,90,90	0

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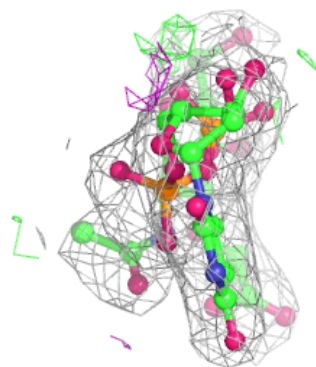
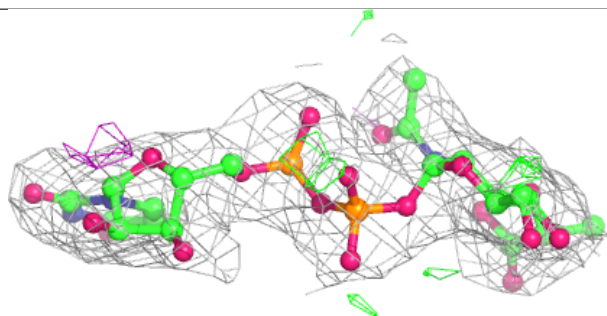
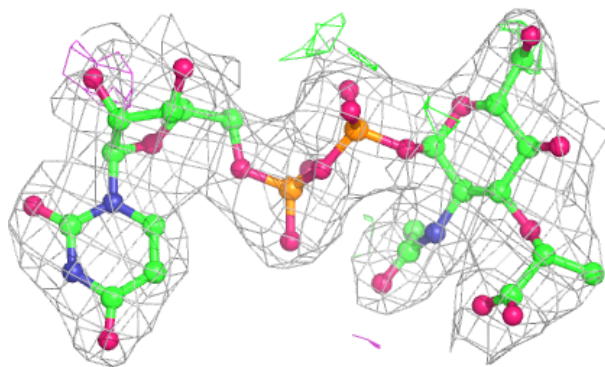
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	B	504	5/5	0.94	0.10	89,90,91,91	0
4	SO4	B	505	5/5	0.95	0.12	88,89,92,92	0
3	EPZ	F	501	44/44	0.96	0.17	56,63,73,77	0
3	EPZ	B	501	44/44	0.96	0.15	51,61,71,72	0
3	EPZ	D	501	44/44	0.97	0.17	51,58,67,74	0
3	EPZ	H	501	44/44	0.97	0.17	52,59,69,74	0
4	SO4	B	503	5/5	0.98	0.11	71,73,74,75	0
4	SO4	F	503	5/5	0.98	0.13	59,59,61,61	0
4	SO4	D	503	5/5	0.98	0.12	54,56,57,58	0
4	SO4	H	503	5/5	0.98	0.12	66,68,70,70	0
4	SO4	D	502	5/5	0.99	0.13	45,45,46,46	0
4	SO4	B	502	5/5	0.99	0.16	48,48,49,49	0
4	SO4	H	502	5/5	0.99	0.15	49,49,51,51	0
4	SO4	F	502	5/5	1.00	0.14	45,46,48,49	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.

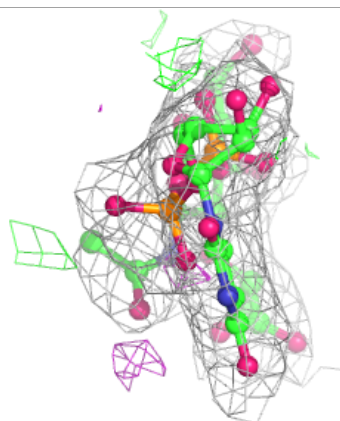
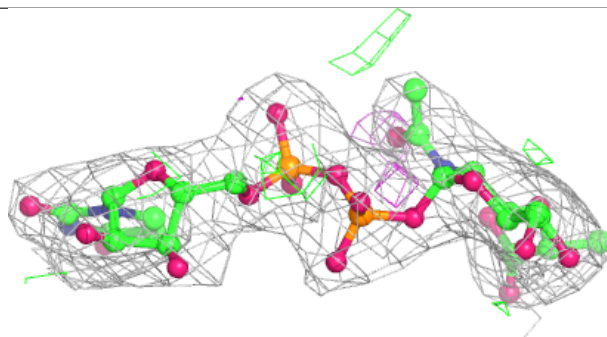
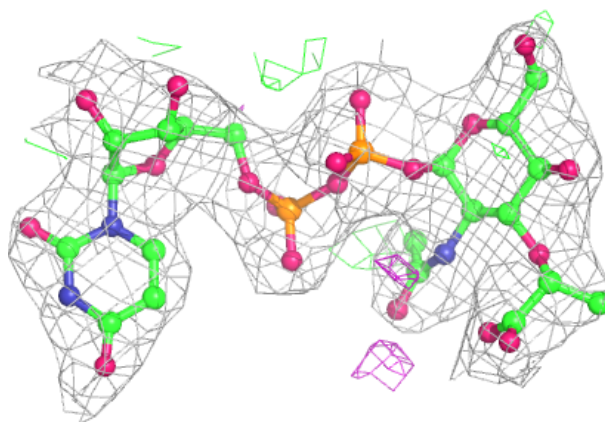


**Electron density around EPZ B 501:**

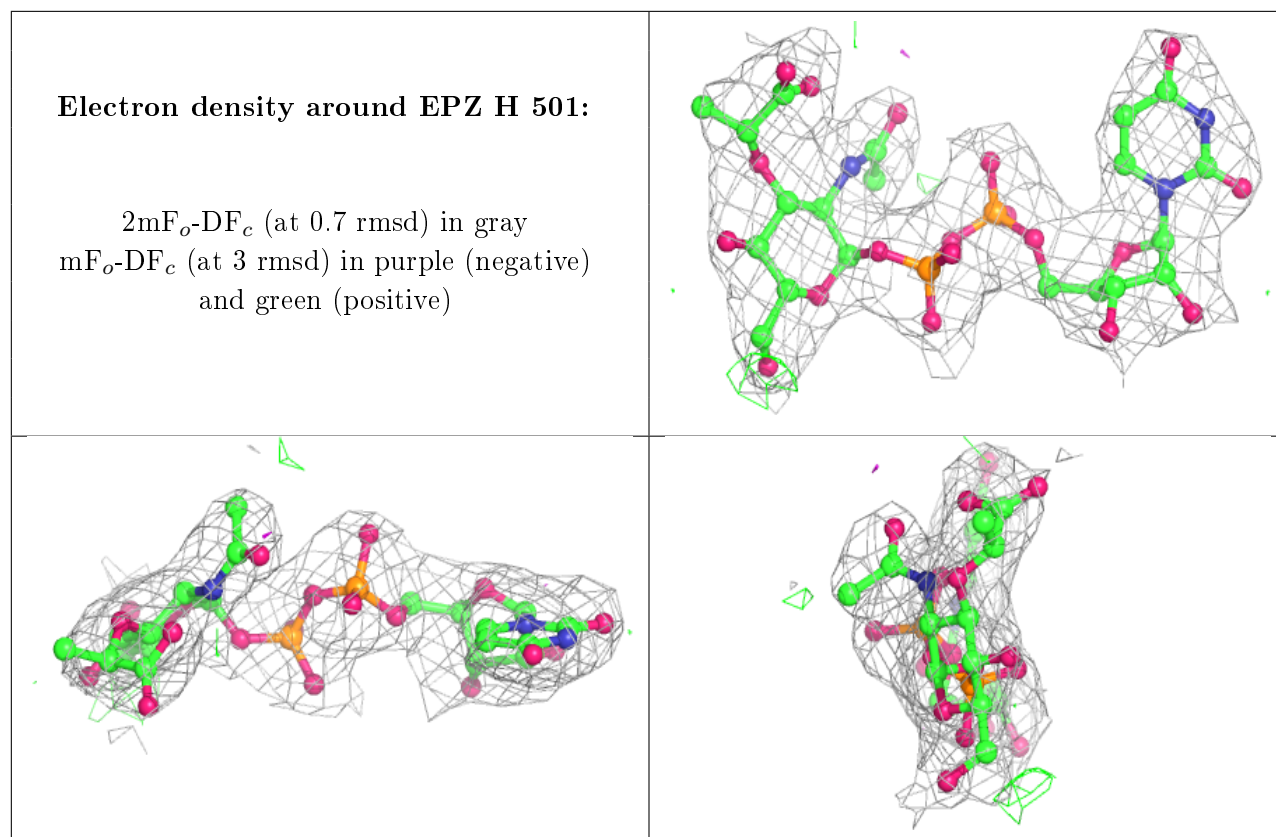
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around EPZ D 501:**

$2mF_o-DF_c$  (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.