



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 07:47 AM EST

PDB ID : 8DHK  
Title : Crystal structure of human Sulfide Quinone Oxidoreductase K207E  
Authors : Mascarenhas, R.N.; Ludlum, A.; Banerjee, R.  
Deposited on : 2022-06-27  
Resolution : 2.30 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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

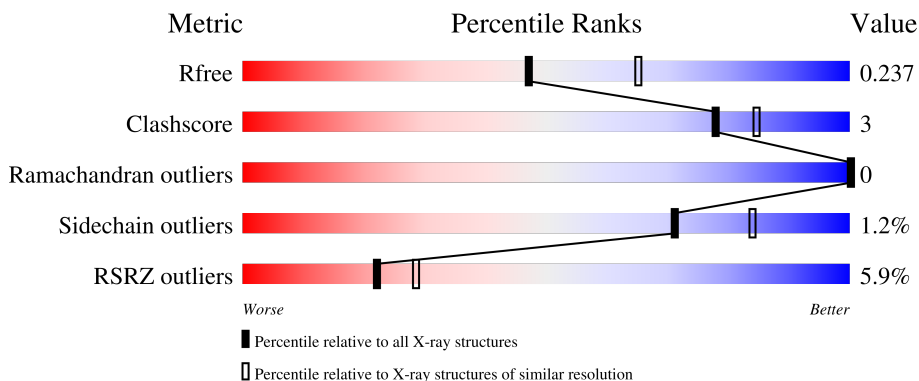
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\geq 3$ , 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	418	 5% 92% 5%
1	B	418	 7% 86% 10%

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
3	PEG	B	506	-	-	-	X
4	MHA	B	507	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13187 atoms, of which 6436 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 Sulfide:quinone oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	406	6282	2023	3121	533	588	17	0	0	0
1	B	405	6281	2021	3127	530	587	16	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	MET	-	initiating methionine	UNP Q9Y6N5
A	207	GLU	LYS	engineered mutation	UNP Q9Y6N5
A	451	LEU	-	expression tag	UNP Q9Y6N5
A	452	GLU	-	expression tag	UNP Q9Y6N5
A	453	HIS	-	expression tag	UNP Q9Y6N5
A	454	HIS	-	expression tag	UNP Q9Y6N5
A	455	HIS	-	expression tag	UNP Q9Y6N5
A	456	HIS	-	expression tag	UNP Q9Y6N5
A	457	HIS	-	expression tag	UNP Q9Y6N5
A	458	HIS	-	expression tag	UNP Q9Y6N5
B	41	MET	-	initiating methionine	UNP Q9Y6N5
B	207	GLU	LYS	engineered mutation	UNP Q9Y6N5
B	451	LEU	-	expression tag	UNP Q9Y6N5
B	452	GLU	-	expression tag	UNP Q9Y6N5
B	453	HIS	-	expression tag	UNP Q9Y6N5
B	454	HIS	-	expression tag	UNP Q9Y6N5
B	455	HIS	-	expression tag	UNP Q9Y6N5
B	456	HIS	-	expression tag	UNP Q9Y6N5
B	457	HIS	-	expression tag	UNP Q9Y6N5
B	458	HIS	-	expression tag	UNP Q9Y6N5

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
2	A	1	84	27	31	9	15	2	0	0
2	B	1	84	27	31	9	15	2	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



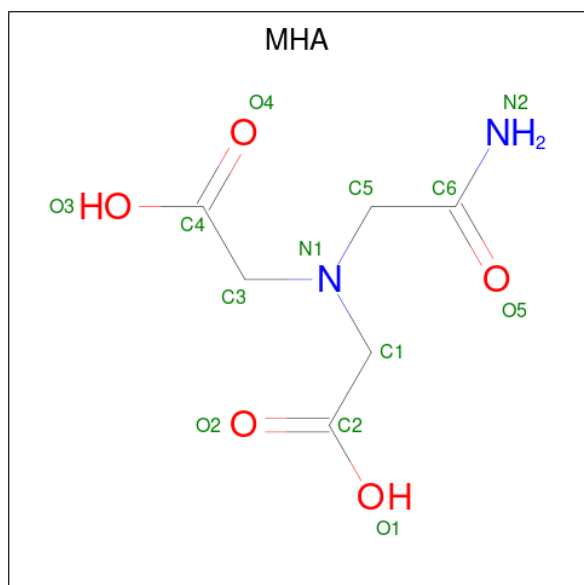
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	H			O
3	A	1	17	4	10	3	0	0
3	A	1	17	4	10	3	0	0

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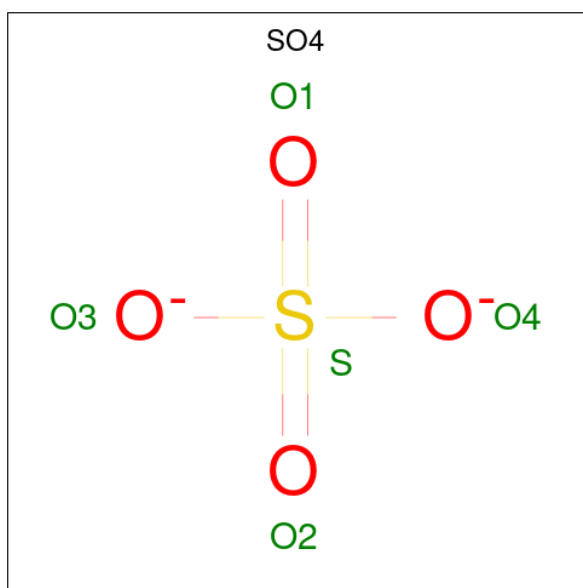
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			17	4	10	3		
3	A	1	Total	C	H	O	0	0
			17	4	10	3		
3	A	1	Total	C	H	O	0	0
			17	4	10	3		
3	B	1	Total	C	H	O	0	0
			17	4	10	3		
3	B	1	Total	C	H	O	0	0
			17	4	10	3		
3	B	1	Total	C	H	O	0	0
			17	4	10	3		
3	B	1	Total	C	H	O	0	0
			17	4	10	3		
3	B	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 4 is (CARBAMOYLMETHYL-CARBOXYMETHYL-AMINO)-ACETIC ACID (three-letter code: MHA) (formula: C<sub>6</sub>H<sub>10</sub>N<sub>2</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	A	1	Total	C	H	N	O	0	0
			21	6	8	2	5		
4	B	1	Total	C	H	N	O	0	0
			21	6	8	2	5		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

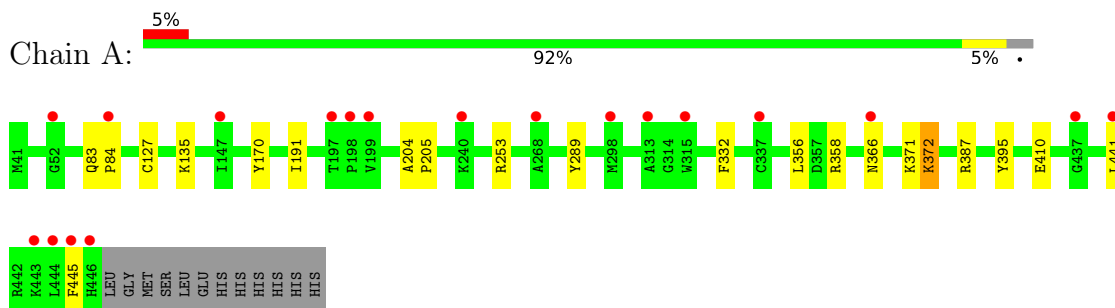
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	103	Total O 103 103	0	0
6	B	104	Total O 104 104	0	0

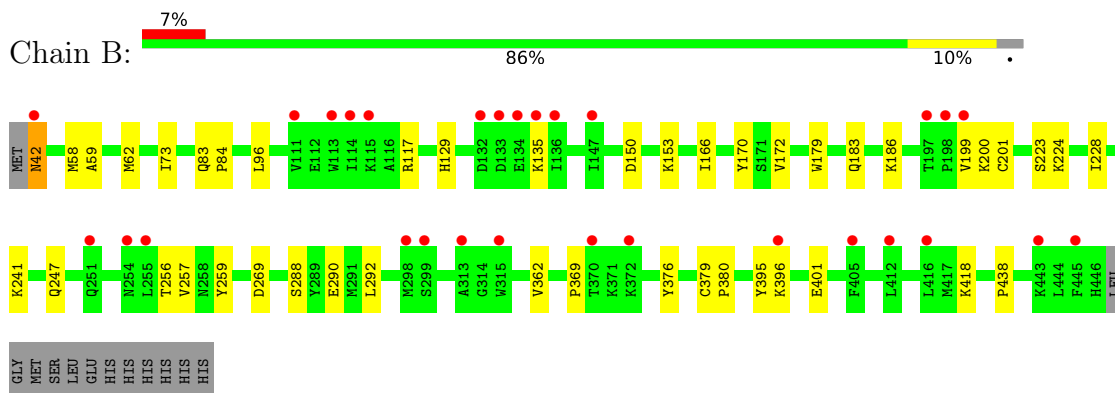
### 3 Residue-property plots [i](#)

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: Sulfide:quinone oxidoreductase



- Molecule 1: Sulfide:quinone oxidoreductase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.79Å 111.30Å 134.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.41 – 2.30 45.06 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (33.41-2.30) 99.8 (45.06-2.30)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.197 , 0.237 0.197 , 0.237	Depositor DCC
$R_{free}$ test set	2662 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.7	Xtrriage
Anisotropy	0.088	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 46.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13187	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: CSS, PEG, MHA, SO4, FAD

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	0.29	0/3229	0.49	0/4384
1	B	0.29	0/3222	0.48	0/4372
All	All	0.29	0/6451	0.49	0/8756

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	3161	3121	3121	14	0
1	B	3154	3127	3125	24	0
2	A	53	31	31	2	0
2	B	53	31	31	2	0
3	A	35	50	50	0	0
3	B	42	60	60	0	0
4	A	13	8	8	0	0
4	B	13	8	8	0	0
5	A	5	0	0	0	0
5	B	15	0	0	0	0
6	A	103	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	104	0	0	2	0
All	All	6751	6436	6434	38	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 3.

All (38) 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:A:127:CYS:SG	1:A:135:LYS:NZ	2.36	0.97
1:A:170:TYR:CD2	2:A:501:FAD:HM83	2.17	0.79
1:B:170:TYR:CD2	2:B:501:FAD:HM83	2.21	0.75
1:B:166:ILE:HD12	1:B:292:LEU:HD23	1.80	0.63
1:B:96:LEU:HD11	1:B:172:VAL:HG23	1.84	0.59
1:B:129:HIS:CE1	1:B:135:LYS:HE2	2.43	0.54
1:B:269:ASP:N	1:B:269:ASP:OD1	2.41	0.54
1:B:150:ASP:HB3	1:B:153:LYS:HG2	1.91	0.52
1:A:191:ILE:HD12	1:A:289:TYR:HB3	1.91	0.52
1:B:186:LYS:HE3	1:B:290:GLU:OE2	2.10	0.52
1:B:228:ILE:HG22	1:B:256:THR:HB	1.93	0.51
1:B:170:TYR:CE2	2:B:501:FAD:HM83	2.47	0.50
1:B:241:LYS:NZ	1:B:401:GLU:OE1	2.43	0.49
1:A:253:ARG:NH1	6:A:603:HOH:O	2.40	0.49
1:B:83:GLN:N	1:B:84:PRO:CD	2.76	0.49
1:B:58:MET:O	1:B:62:MET:HG2	2.14	0.48
1:B:129:HIS:CE1	1:B:135:LYS:HZ3	2.32	0.48
1:A:371:LYS:HD2	1:A:371:LYS:H	1.78	0.47
1:A:332:PHE:HB3	1:A:356:LEU:HD11	1.97	0.46
1:A:170:TYR:CE2	2:A:501:FAD:HM83	2.49	0.45
1:A:372:LYS:NZ	6:A:607:HOH:O	2.49	0.44
1:A:387:ARG:HB3	1:A:410:GLU:HB3	1.98	0.44
1:B:380:PRO:O	1:B:418:LYS:HE3	2.17	0.44
1:B:223:SER:HB2	1:B:224:LYS:HE2	1.99	0.44
1:A:441:LEU:HD23	1:A:441:LEU:N	2.33	0.43
1:B:362:VAL:HG21	1:B:369:PRO:HA	1.99	0.43
1:B:376:TYR:CZ	1:B:438:PRO:HG3	2.54	0.43
1:B:179:TRP:O	1:B:183:GLN:HG3	2.19	0.42
1:B:201:CSS:SD	1:B:379:CYS:SG	2.96	0.42
1:A:204:ALA:N	1:A:205:PRO:CD	2.82	0.42
1:A:83:GLN:N	1:A:84:PRO:CD	2.82	0.42
1:B:42:ASN:ND2	6:B:612:HOH:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:PHE:N	1:A:445:PHE:CD2	2.87	0.41
1:B:199:VAL:HG12	1:B:200:LYS:O	2.20	0.41
1:B:257:VAL:HG11	1:B:259:TYR:CZ	2.55	0.41
1:B:59:ALA:CB	1:B:73:ILE:HD11	2.51	0.41
1:B:247:GLN:NE2	6:B:604:HOH:O	2.46	0.41
1:A:358:ARG:HB3	1:A:371:LYS:HD3	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	403/418 (96%)	393 (98%)	10 (2%)	0	100	100
1	B	402/418 (96%)	387 (96%)	15 (4%)	0	100	100
All	All	805/836 (96%)	780 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	333/354 (94%)	330 (99%)	3 (1%)	78	89
1	B	333/354 (94%)	328 (98%)	5 (2%)	65	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	666/708 (94%)	658 (99%)	8 (1%)	71 84

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	366	ASN
1	A	372	LYS
1	A	395	TYR
1	B	42	ASN
1	B	117	ARG
1	B	288	SER
1	B	395	TYR
1	B	396	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 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	$\# Z  > 2$
1	CSS	B	201	1	4,6,7	0.99	0	1,6,8	0.12	0
1	CSS	A	201	1	4,6,7	1.09	0	1,6,8	0.72	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
1	CSS	B	201	1	-	0/1/5/7	-
1	CSS	A	201	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	201	CSS	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

19 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	FAD	A	501	-	53,58,58	0.55	0	68,89,89	0.57	1 (1%)
3	PEG	A	504	-	6,6,6	0.48	0	5,5,5	0.64	0
5	SO4	B	510	-	4,4,4	0.14	0	6,6,6	0.05	0
3	PEG	B	506	-	6,6,6	0.49	0	5,5,5	0.28	0
3	PEG	A	502	-	6,6,6	0.49	0	5,5,5	0.28	0
5	SO4	B	509	-	4,4,4	0.14	0	6,6,6	0.09	0
3	PEG	B	504	-	6,6,6	0.47	0	5,5,5	0.36	0
3	PEG	B	503	-	6,6,6	0.48	0	5,5,5	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PEG	B	511	-	6,6,6	0.48	0	5,5,5	0.32	0
4	MHA	B	507	-	12,12,12	1.53	1 (8%)	15,15,15	1.42	2 (13%)
3	PEG	B	502	-	6,6,6	0.49	0	5,5,5	0.39	0
3	PEG	A	507	-	6,6,6	0.49	0	5,5,5	0.32	0
3	PEG	A	505	-	6,6,6	0.49	0	5,5,5	0.28	0
3	PEG	A	508	-	6,6,6	0.49	0	5,5,5	0.44	0
5	SO4	B	508	-	4,4,4	0.15	0	6,6,6	0.12	0
3	PEG	B	505	-	6,6,6	0.49	0	5,5,5	0.33	0
5	SO4	A	506	-	4,4,4	0.14	0	6,6,6	0.09	0
2	FAD	B	501	-	53,58,58	0.56	0	68,89,89	0.58	1 (1%)
4	MHA	A	503	-	12,12,12	1.63	1 (8%)	15,15,15	1.57	2 (13%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	B	505	-	-	2/4/4/4	-
3	PEG	B	504	-	-	3/4/4/4	-
3	PEG	B	503	-	-	2/4/4/4	-
2	FAD	A	501	-	-	1/30/50/50	0/6/6/6
3	PEG	A	507	-	-	3/4/4/4	-
3	PEG	B	511	-	-	2/4/4/4	-
2	FAD	B	501	-	-	2/30/50/50	0/6/6/6
4	MHA	B	507	-	-	7/12/12/12	-
3	PEG	B	502	-	-	4/4/4/4	-
3	PEG	A	504	-	-	4/4/4/4	-
4	MHA	A	503	-	-	4/12/12/12	-
3	PEG	B	506	-	-	0/4/4/4	-
3	PEG	A	502	-	-	2/4/4/4	-
3	PEG	A	505	-	-	4/4/4/4	-
3	PEG	A	508	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	MHA	C6-N2	4.16	1.46	1.32
4	B	507	MHA	C6-N2	3.93	1.45	1.32

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	MHA	C5-C6-N2	3.54	121.45	115.86
4	B	507	MHA	C5-C6-N2	3.09	120.73	115.86
4	B	507	MHA	C6-C5-N1	-2.41	110.20	114.38
2	B	501	FAD	C5A-C6A-N6A	2.38	123.97	120.35
2	A	501	FAD	C5A-C6A-N6A	2.32	123.87	120.35
4	A	503	MHA	C5-N1-C1	2.03	116.12	111.54

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	507	MHA	N1-C1-C2-O2
4	B	507	MHA	N1-C3-C4-O3
4	B	507	MHA	N1-C3-C4-O4
4	B	507	MHA	N1-C1-C2-O1
4	A	503	MHA	C2-C1-N1-C5
3	A	504	PEG	C1-C2-O2-C3
3	A	505	PEG	O2-C3-C4-O4
3	A	507	PEG	O1-C1-C2-O2
3	A	507	PEG	O2-C3-C4-O4
3	B	502	PEG	O1-C1-C2-O2
3	A	502	PEG	O2-C3-C4-O4
3	B	511	PEG	O2-C3-C4-O4
3	A	502	PEG	O1-C1-C2-O2
3	A	504	PEG	O1-C1-C2-O2
3	A	508	PEG	O1-C1-C2-O2
3	B	504	PEG	O1-C1-C2-O2
3	B	504	PEG	O2-C3-C4-O4
4	A	503	MHA	N1-C3-C4-O3
3	A	504	PEG	O2-C3-C4-O4
4	A	503	MHA	N1-C3-C4-O4
4	A	503	MHA	C4-C3-N1-C5
3	A	505	PEG	C1-C2-O2-C3
4	B	507	MHA	N1-C5-C6-O5
3	B	505	PEG	O2-C3-C4-O4
3	B	502	PEG	C4-C3-O2-C2
3	B	505	PEG	C1-C2-O2-C3
3	B	504	PEG	C4-C3-O2-C2
3	B	503	PEG	O2-C3-C4-O4
3	A	504	PEG	C4-C3-O2-C2
3	B	503	PEG	C1-C2-O2-C3

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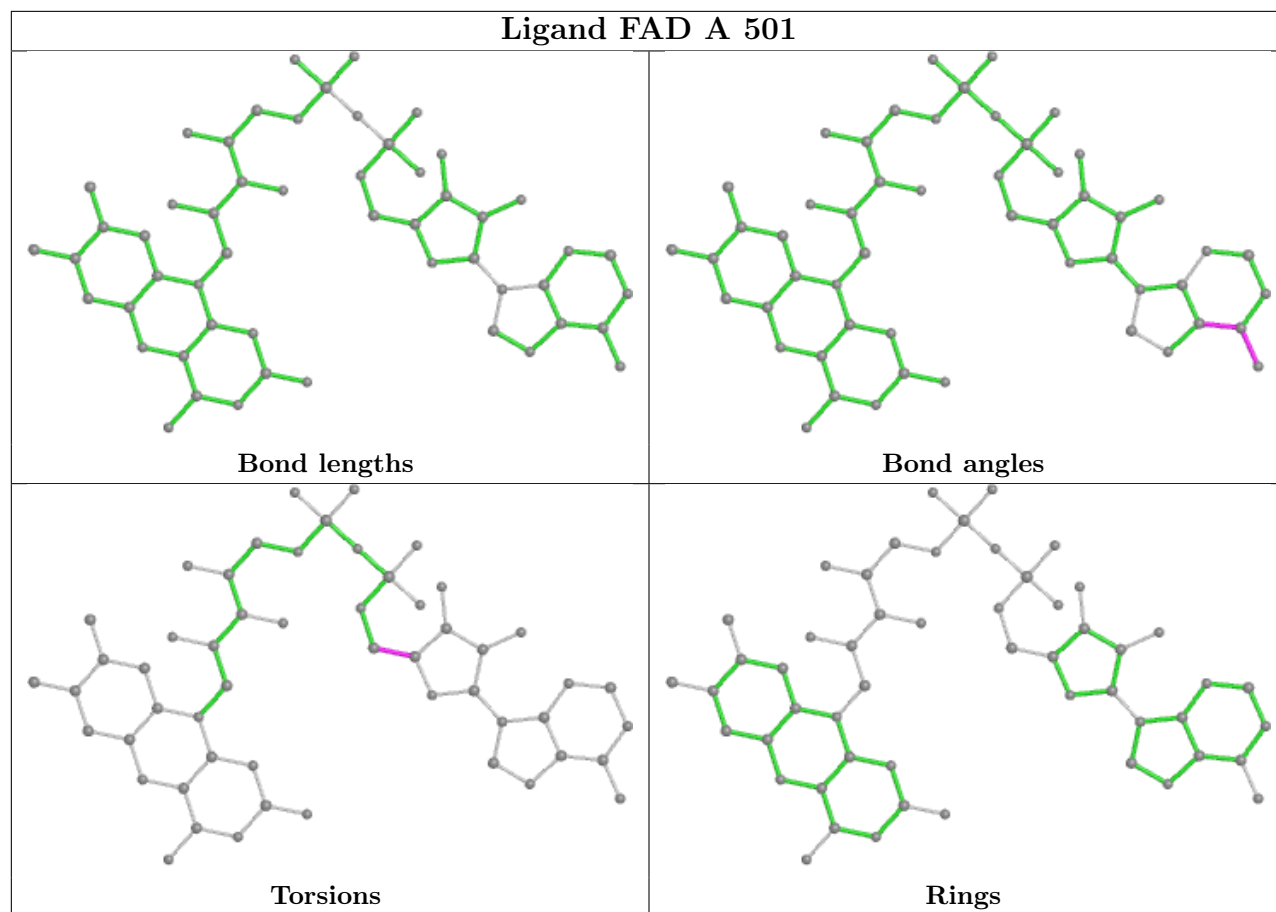
Mol	Chain	Res	Type	Atoms
3	B	511	PEG	C4-C3-O2-C2
4	B	507	MHA	C4-C3-N1-C5
3	A	507	PEG	C1-C2-O2-C3
4	B	507	MHA	N1-C5-C6-N2
3	A	505	PEG	C4-C3-O2-C2
3	A	508	PEG	O2-C3-C4-O4
2	B	501	FAD	O4B-C4B-C5B-O5B
3	A	505	PEG	O1-C1-C2-O2
2	A	501	FAD	O4B-C4B-C5B-O5B
3	B	502	PEG	O2-C3-C4-O4
3	B	502	PEG	C1-C2-O2-C3
2	B	501	FAD	O4'-C4'-C5'-O5'

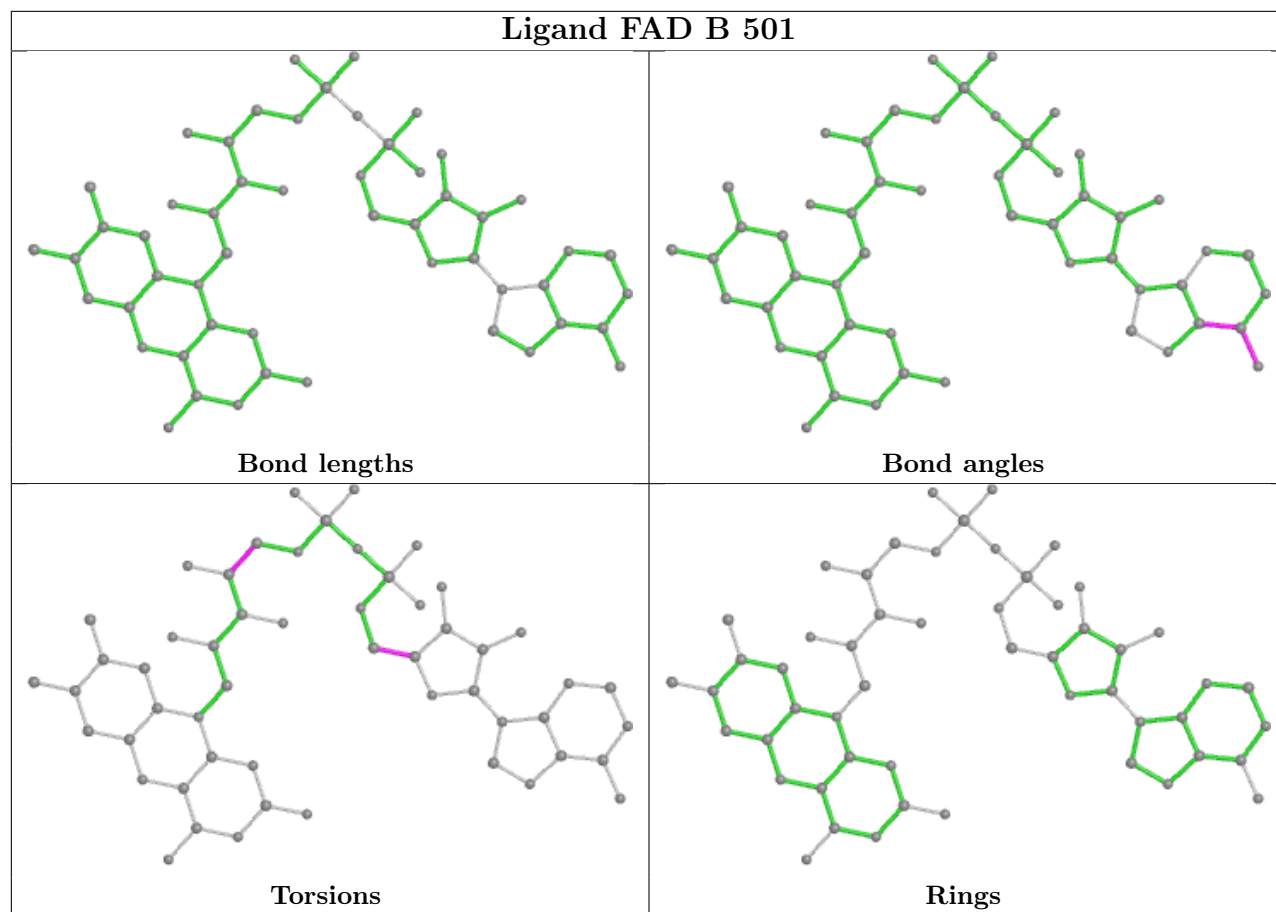
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FAD	2	0
2	B	501	FAD	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	405/418 (96%)	0.25	19 (4%) 31 38	32, 43, 61, 79	0
1	B	404/418 (96%)	0.35	29 (7%) 15 20	34, 47, 68, 81	0
All	All	809/836 (96%)	0.30	48 (5%) 22 28	32, 45, 66, 81	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	445	PHE	8.3
1	A	441	LEU	7.2
1	A	446	HIS	5.2
1	B	133	ASP	4.7
1	A	444	LEU	4.2
1	B	134	GLU	4.2
1	B	298	MET	3.8
1	A	313	ALA	3.8
1	B	115	LYS	3.4
1	B	370	THR	3.4
1	A	298	MET	3.3
1	A	443	LYS	3.2
1	B	445	PHE	3.0
1	B	197	THR	3.0
1	B	412	LEU	2.9
1	B	372	LYS	2.9
1	A	52	GLY	2.8
1	B	198	PRO	2.8
1	B	135	LYS	2.8
1	B	254	ASN	2.7
1	B	405	PHE	2.6
1	A	198	PRO	2.6
1	B	416	LEU	2.5
1	B	313	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	337	CYS	2.5
1	B	42	ASN	2.5
1	A	197	THR	2.5
1	B	136	ILE	2.4
1	B	147	ILE	2.4
1	A	268	ALA	2.4
1	B	113	TRP	2.4
1	B	114	ILE	2.4
1	B	111	VAL	2.4
1	A	366	ASN	2.3
1	A	147	ILE	2.3
1	A	315	TRP	2.2
1	B	396	LYS	2.2
1	B	443	LYS	2.2
1	A	84	PRO	2.2
1	B	132	ASP	2.2
1	A	437	GLY	2.2
1	B	251	GLN	2.1
1	A	240	LYS	2.1
1	B	299	SER	2.1
1	B	199	VAL	2.1
1	B	315	TRP	2.1
1	A	199	VAL	2.0
1	B	255	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
1	CSS	A	201	7/8	0.97	0.22	33,39,49,59	0
1	CSS	B	201	7/8	0.97	0.16	43,46,60,72	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands

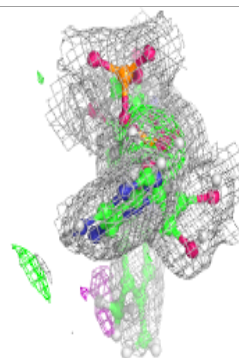
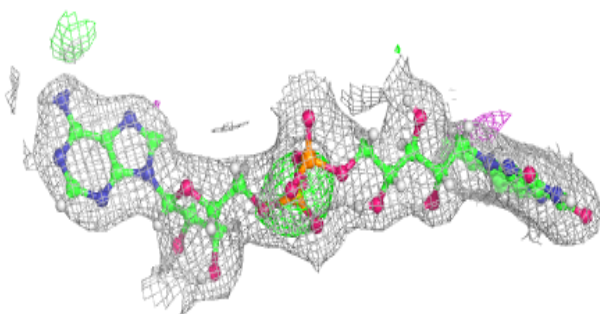
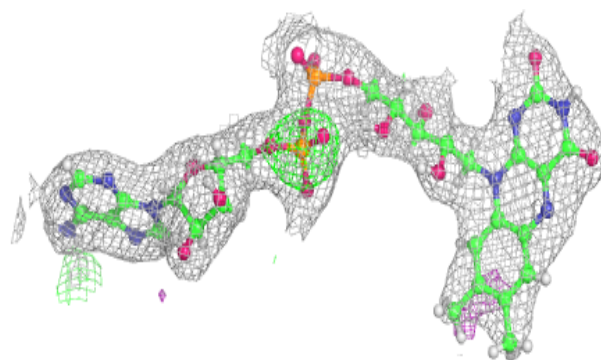
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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
3	PEG	B	506	7/7	0.66	0.56	71,86,96,96	0
5	SO4	B	510	5/5	0.67	0.24	91,107,138,138	0
4	MHA	B	507	13/13	0.71	0.58	72,91,106,110	0
3	PEG	B	502	7/7	0.71	0.17	62,74,84,84	0
3	PEG	A	508	7/7	0.74	0.20	60,72,92,92	0
4	MHA	A	503	13/13	0.74	0.18	44,58,66,68	0
3	PEG	A	505	7/7	0.76	0.32	58,69,98,98	0
3	PEG	B	505	7/7	0.84	0.41	67,80,94,94	0
3	PEG	B	503	7/7	0.86	0.27	65,79,95,113	0
5	SO4	B	509	5/5	0.88	0.18	70,73,94,95	0
3	PEG	A	507	7/7	0.88	0.35	63,75,86,87	0
5	SO4	A	506	5/5	0.89	0.14	64,70,100,103	0
3	PEG	B	504	7/7	0.90	0.31	51,69,89,91	0
3	PEG	A	504	7/7	0.90	0.26	53,64,77,77	0
3	PEG	B	511	7/7	0.91	0.12	68,81,95,95	0
3	PEG	A	502	7/7	0.91	0.14	52,63,73,76	0
2	FAD	B	501	53/53	0.91	0.18	31,46,55,129	0
5	SO4	B	508	5/5	0.94	0.11	55,67,74,89	0
2	FAD	A	501	53/53	0.95	0.23	27,39,49,67	0

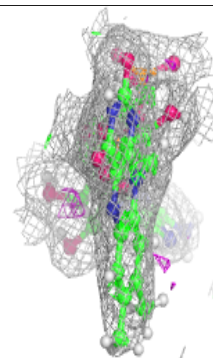
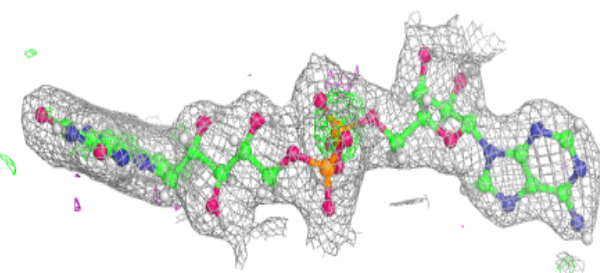
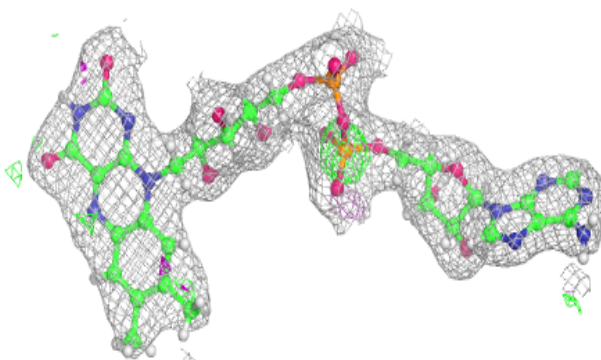
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around FAD 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 FAD A 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.