



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 7, 2022 – 05:02 PM JST

PDB ID : 8HDD
Title : Complex structure of catalytic, small, and a partial electron transfer subunits from Burkholderia cepacia FAD glucose dehydrogenase
Authors : Yoshida, H.; Sode, K.
Deposited on : 2022-11-04
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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
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)	:	2.31.3

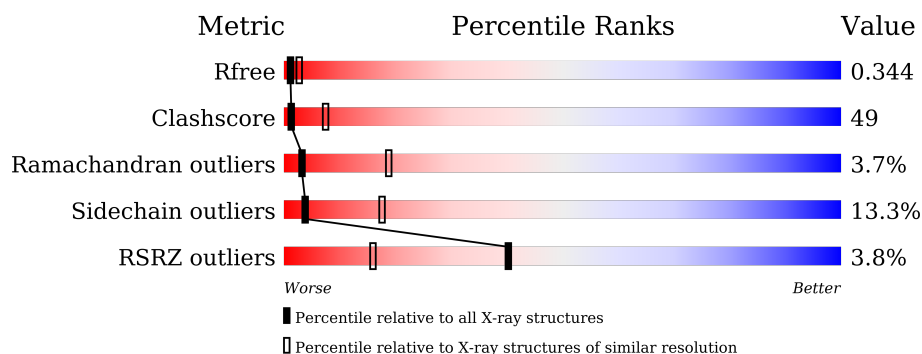
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 $\leq 5\%$. 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	539	
2	B	482	
3	C	121	

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	F3S	A	702	-	-	X	-
6	HEM	B	501	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6037 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 Glucose dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	530	Total	C	N	O	S	0	0	0
			4145	2628	725	770	22			

- Molecule 2 is a protein called Glucose dehydrogenase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	121	Total	C	N	O	S	0	0	0
			899	560	161	174	4			

There are 59 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2	GLY	ARG	engineered mutation	UNP Q71JE9
B	136	VAL	ALA	engineered mutation	UNP Q71JE9
B	426	SER	-	expression tag	UNP Q71JE9
B	427	GLY	-	expression tag	UNP Q71JE9
B	428	GLY	-	expression tag	UNP Q71JE9
B	429	PRO	-	expression tag	UNP Q71JE9
B	430	VAL	-	expression tag	UNP Q71JE9
B	431	PRO	-	expression tag	UNP Q71JE9
B	432	LEU	-	expression tag	UNP Q71JE9
B	433	LEU	-	expression tag	UNP Q71JE9
B	434	VAL	-	expression tag	UNP Q71JE9
B	435	ARG	-	expression tag	UNP Q71JE9
B	436	VAL	-	expression tag	UNP Q71JE9
B	437	ARG	-	expression tag	UNP Q71JE9
B	438	PRO	-	expression tag	UNP Q71JE9
B	439	LEU	-	expression tag	UNP Q71JE9
B	440	MET	-	expression tag	UNP Q71JE9
B	441	LEU	-	expression tag	UNP Q71JE9
B	442	PRO	-	expression tag	UNP Q71JE9
B	443	GLY	-	expression tag	UNP Q71JE9

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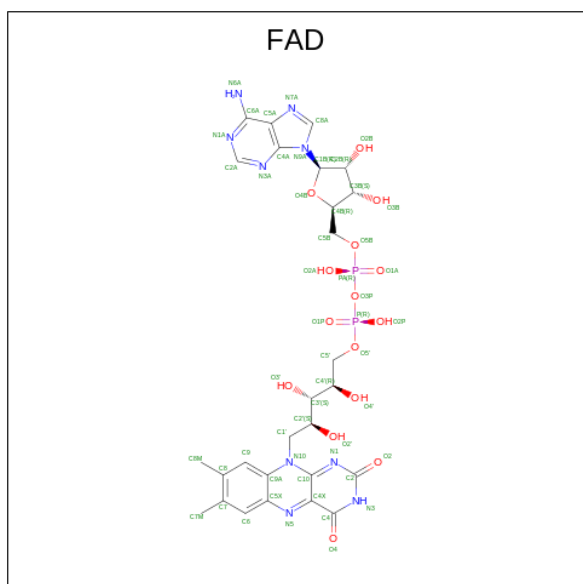
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Chain	Residue	Modelled	Actual	Comment	Reference
B	444	ALA	-	expression tag	UNP Q71JE9
B	445	VAL	-	expression tag	UNP Q71JE9
B	446	VAL	-	expression tag	UNP Q71JE9
B	447	VAL	-	expression tag	UNP Q71JE9
B	448	VAL	-	expression tag	UNP Q71JE9
B	449	LEU	-	expression tag	UNP Q71JE9
B	450	ILE	-	expression tag	UNP Q71JE9
B	451	ALA	-	expression tag	UNP Q71JE9
B	452	LEU	-	expression tag	UNP Q71JE9
B	453	LEU	-	expression tag	UNP Q71JE9
B	454	GLY	-	expression tag	UNP Q71JE9
B	455	VAL	-	expression tag	UNP Q71JE9
B	456	ALA	-	expression tag	UNP Q71JE9
B	457	PHE	-	expression tag	UNP Q71JE9
B	458	TRP	-	expression tag	UNP Q71JE9
B	459	TRP	-	expression tag	UNP Q71JE9
B	460	ARG	-	expression tag	UNP Q71JE9
B	461	ARG	-	expression tag	UNP Q71JE9
B	462	ARG	-	expression tag	UNP Q71JE9
B	463	GLN	-	expression tag	UNP Q71JE9
B	464	ARG	-	expression tag	UNP Q71JE9
B	465	THR	-	expression tag	UNP Q71JE9
B	466	PRO	-	expression tag	UNP Q71JE9
B	467	LEU	-	expression tag	UNP Q71JE9
B	468	ALA	-	expression tag	UNP Q71JE9
B	469	ASN	-	expression tag	UNP Q71JE9
B	470	PRO	-	expression tag	UNP Q71JE9
B	471	PRO	-	expression tag	UNP Q71JE9
B	472	GLN	-	expression tag	UNP Q71JE9
B	473	GLY	-	expression tag	UNP Q71JE9
B	474	LYS	-	expression tag	UNP Q71JE9
B	475	ALA	-	expression tag	UNP Q71JE9
B	476	GLY	-	expression tag	UNP Q71JE9
B	477	HIS	-	expression tag	UNP Q71JE9
B	478	HIS	-	expression tag	UNP Q71JE9
B	479	HIS	-	expression tag	UNP Q71JE9
B	480	HIS	-	expression tag	UNP Q71JE9
B	481	HIS	-	expression tag	UNP Q71JE9
B	482	HIS	-	expression tag	UNP Q71JE9

- Molecule 3 is a protein called Twin-arginine translocation pathway signal.

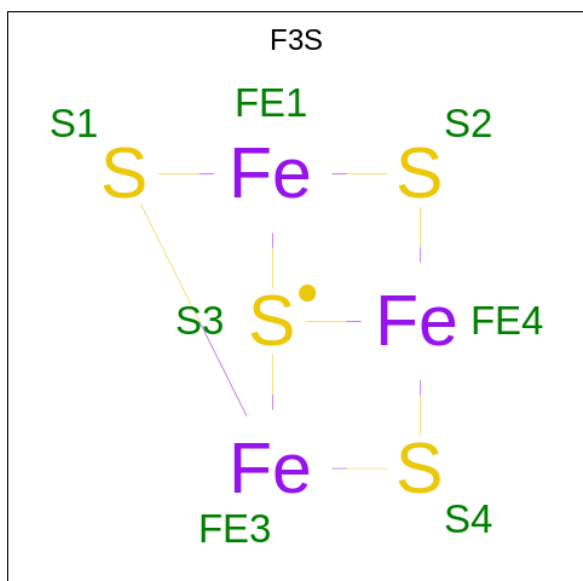
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	117	Total	C	N	O	S	0	0	0
			890	571	144	172	3			

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



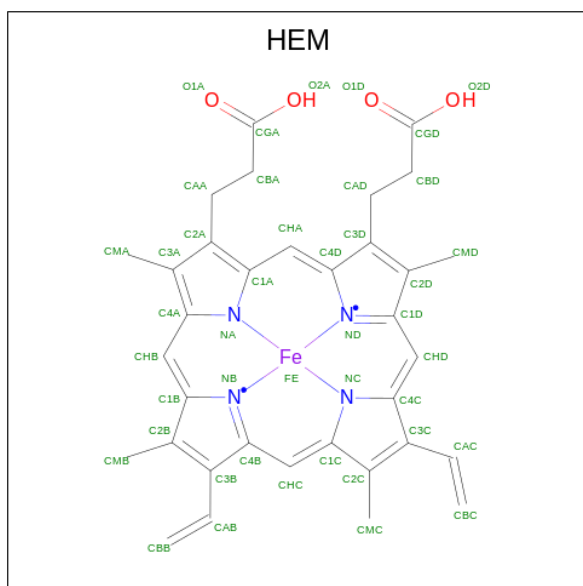
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

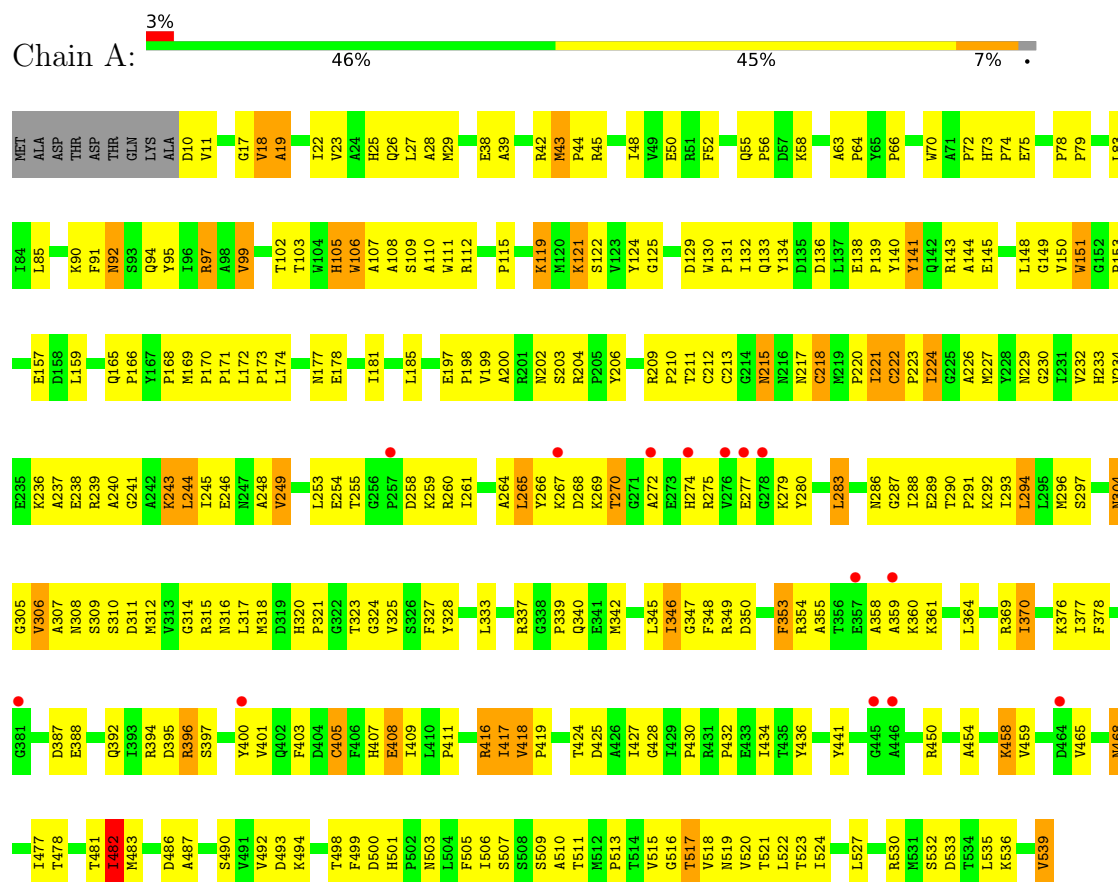


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

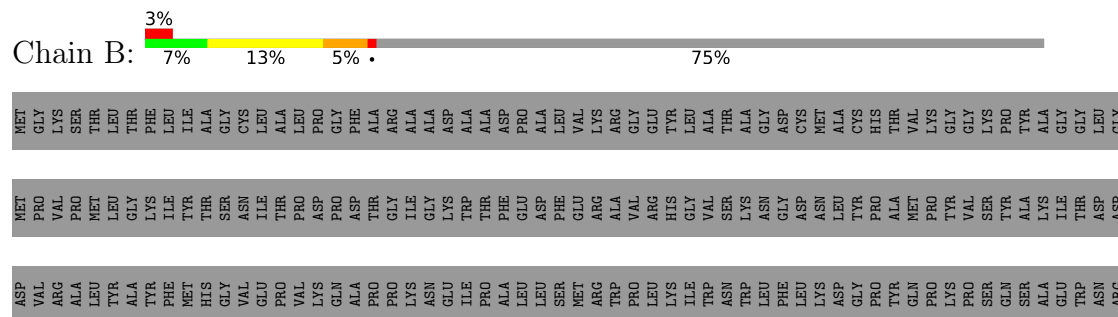
3 Residue-property plots

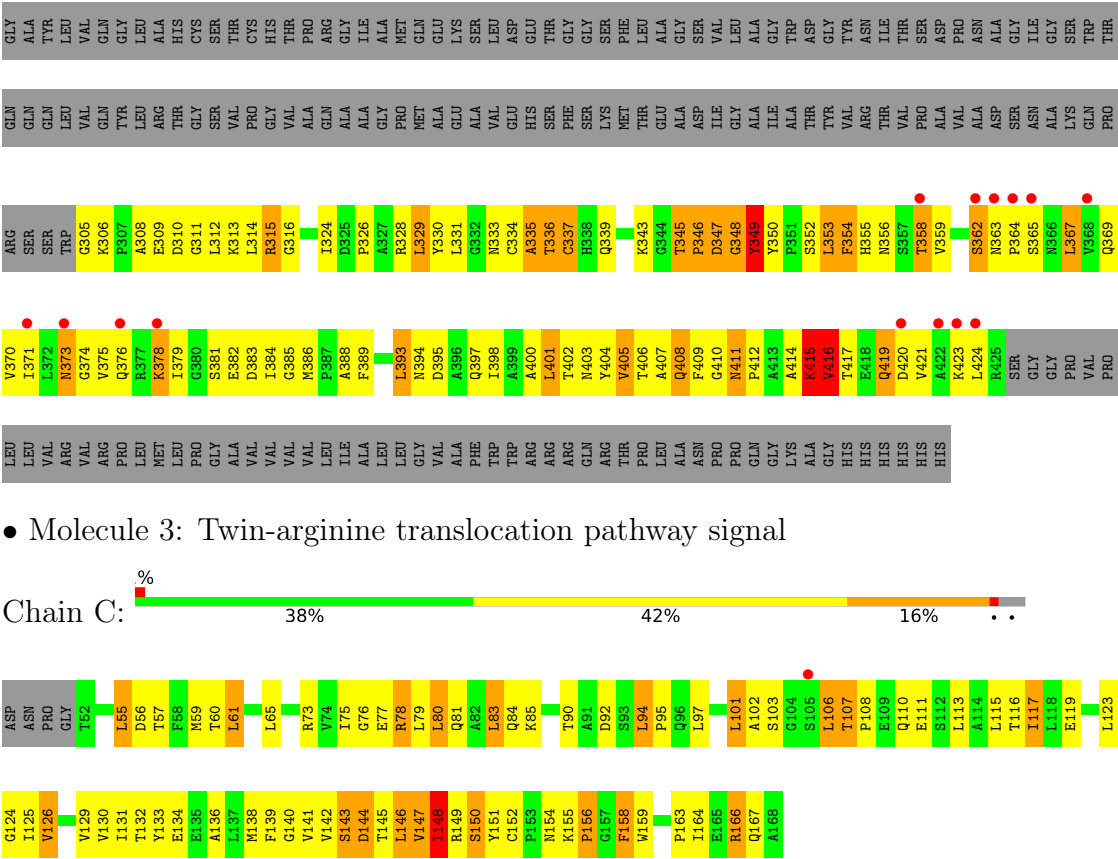
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glucose dehydrogenase



• Molecule 2: Glucose dehydrogenase beta subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	204.01Å 71.80Å 114.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.88 – 3.00 49.83 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.88-3.00) 99.8 (49.83-3.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.275 , 0.323 0.303 , 0.344	Depositor DCC
R_{free} test set	1725 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	53.6	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , -10.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	6037	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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: F3S, HEM, 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	0.63	0/4256	0.67	0/5788
2	B	0.65	0/915	0.71	0/1241
3	C	0.65	0/906	0.69	0/1231
All	All	0.64	0/6077	0.68	0/8260

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

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	4145	0	4067	345	0
2	B	899	0	888	137	0
3	C	890	0	907	144	0
4	A	53	0	30	10	0
5	A	7	0	0	4	0
6	B	43	0	30	25	0
All	All	6037	0	5922	586	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 49.

The worst 5 of 586 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:280:TYR:CE1	1:A:539:VAL:HG13	1.64	1.32
2:B:408:GLN:O	2:B:408:GLN:NE2	1.67	1.28
2:B:369:GLN:NE2	2:B:424:LEU:HD13	1.53	1.21
3:C:107:THR:HG23	3:C:110:GLN:HB2	1.28	1.16
1:A:394:ARG:CG	3:C:142:VAL:HG22	1.76	1.15

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	528/539 (98%)	466 (88%)	51 (10%)	11 (2%)	7	33
2	B	119/482 (25%)	82 (69%)	26 (22%)	11 (9%)	1	3
3	C	115/121 (95%)	92 (80%)	17 (15%)	6 (5%)	2	12
All	All	762/1142 (67%)	640 (84%)	94 (12%)	28 (4%)	3	19

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	259	LYS
2	B	335	ALA
2	B	346	PRO
2	B	347	ASP
2	B	348	GLY

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	441/448 (98%)	399 (90%)	42 (10%)	8	32
2	B	94/376 (25%)	69 (73%)	25 (27%)	0	2
3	C	97/100 (97%)	80 (82%)	17 (18%)	2	10
All	All	632/924 (68%)	548 (87%)	84 (13%)	4	17

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	376	GLN
3	C	94	LEU
2	B	384	ILE
2	B	416	VAL
3	C	115	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	403	ASN
3	C	81	GLN
3	C	84	GLN
2	B	419	GLN
2	B	333	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	HEM	B	501	2	41,50,50	1.32	5 (12%)	45,82,82	1.74	10 (22%)
5	F3S	A	702	1	0,9,9	-	-	-	-	-
4	FAD	A	701	1	53,58,58	0.61	0	68,89,89	0.69	2 (2%)

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	F3S	A	702	1	-	-	0/3/3/3
6	HEM	B	501	2	-	6/12/54/54	-
4	FAD	A	701	1	-	3/30/50/50	0/6/6/6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	501	HEM	C1B-NB	-3.15	1.34	1.40
6	B	501	HEM	C4D-ND	-3.12	1.34	1.40
6	B	501	HEM	FE-NB	2.95	2.11	1.96
6	B	501	HEM	CHB-C1B	2.13	1.40	1.35
6	B	501	HEM	C3B-C4B	2.10	1.49	1.44

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	501	HEM	CHC-C4B-NB	4.69	129.52	124.43
6	B	501	HEM	CHD-C1D-ND	3.86	128.62	124.43
6	B	501	HEM	C1B-NB-C4B	3.72	108.91	105.07
6	B	501	HEM	CHA-C4D-ND	3.49	128.69	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	501	HEM	CHB-C1B-NB	3.42	128.61	124.38

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

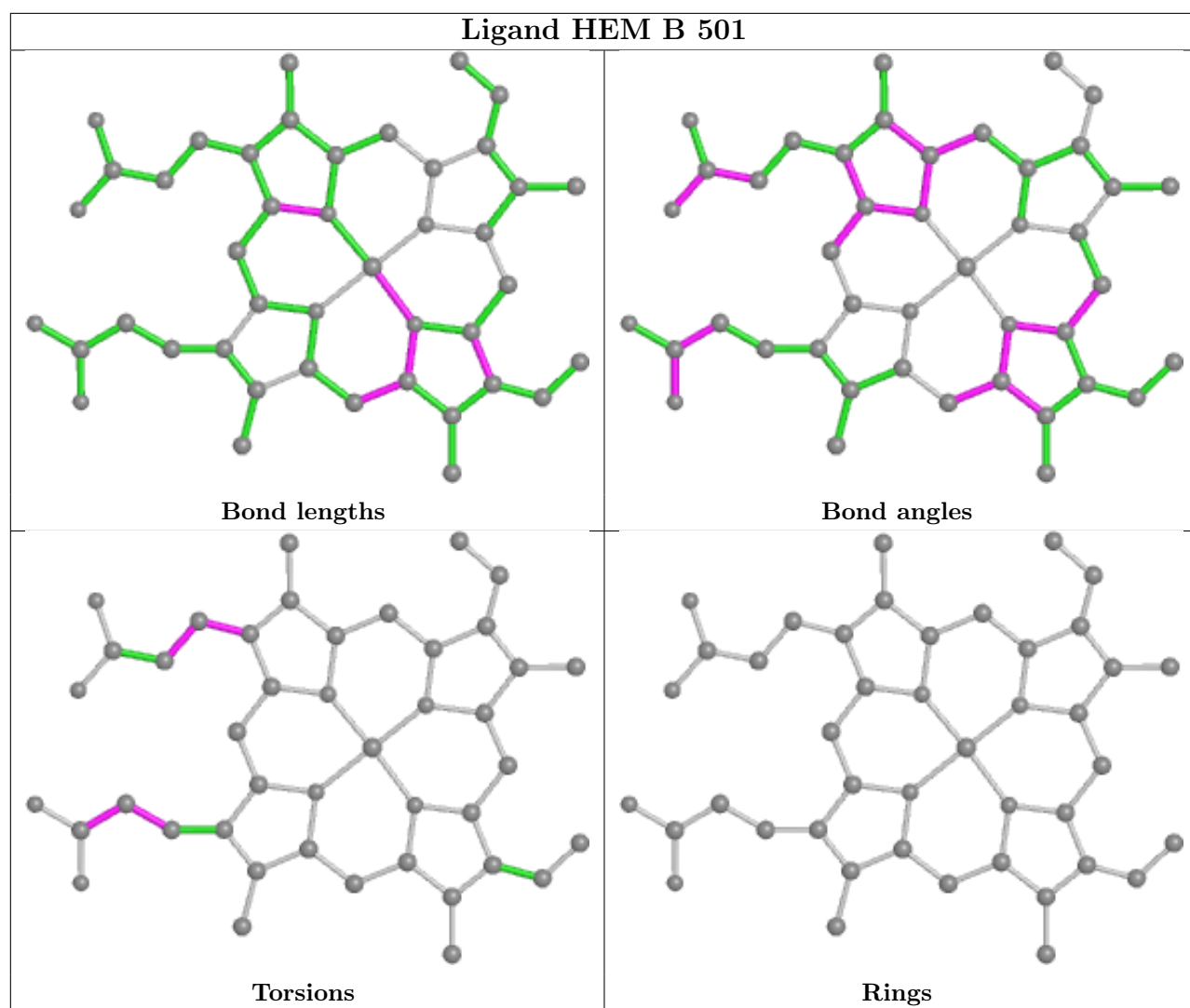
Mol	Chain	Res	Type	Atoms
6	B	501	HEM	C2A-CAA-CBA-CGA
6	B	501	HEM	C3D-CAD-CBD-CGD
6	B	501	HEM	C2D-C3D-CAD-CBD
6	B	501	HEM	C4D-C3D-CAD-CBD
4	A	701	FAD	PA-O3P-P-O5'

There are no ring outliers.

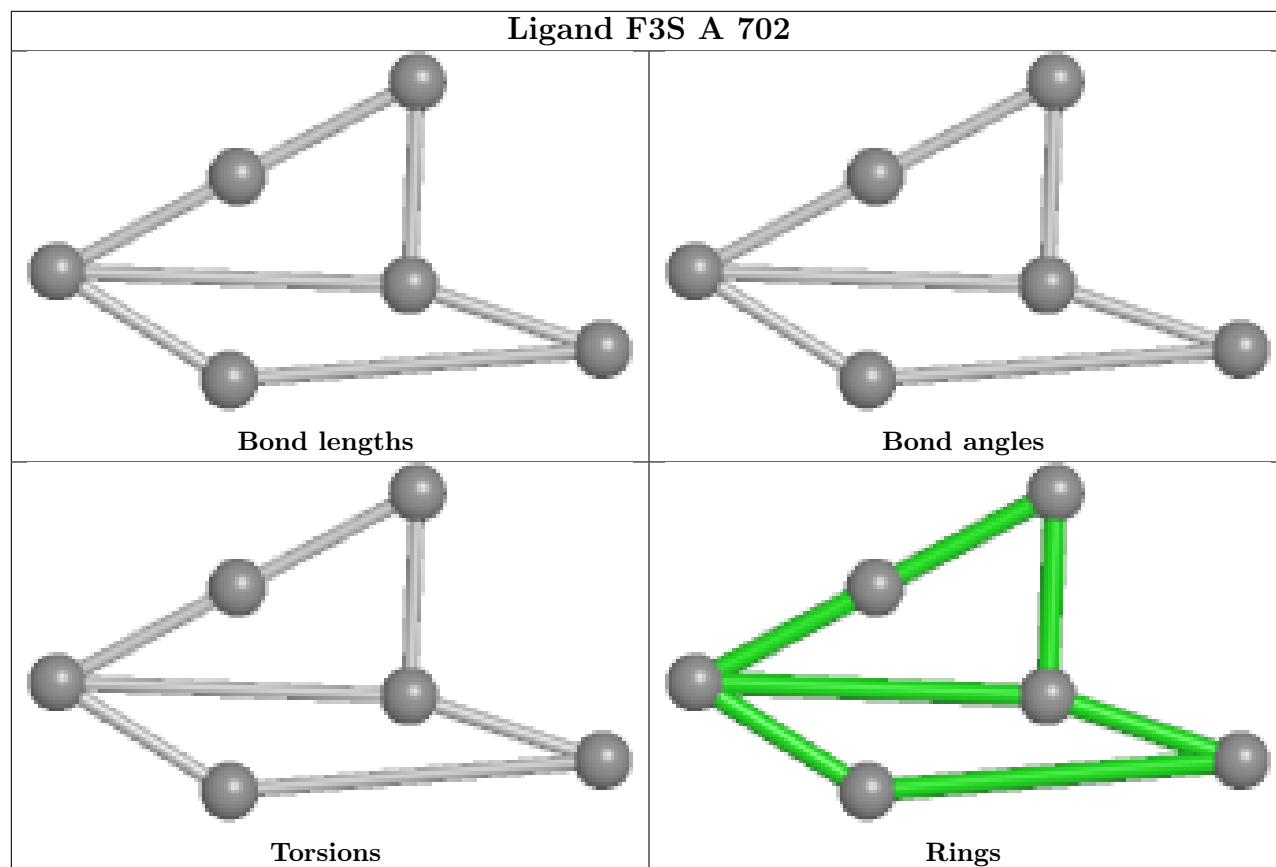
3 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	501	HEM	25	0
5	A	702	F3S	4	0
4	A	701	FAD	10	0

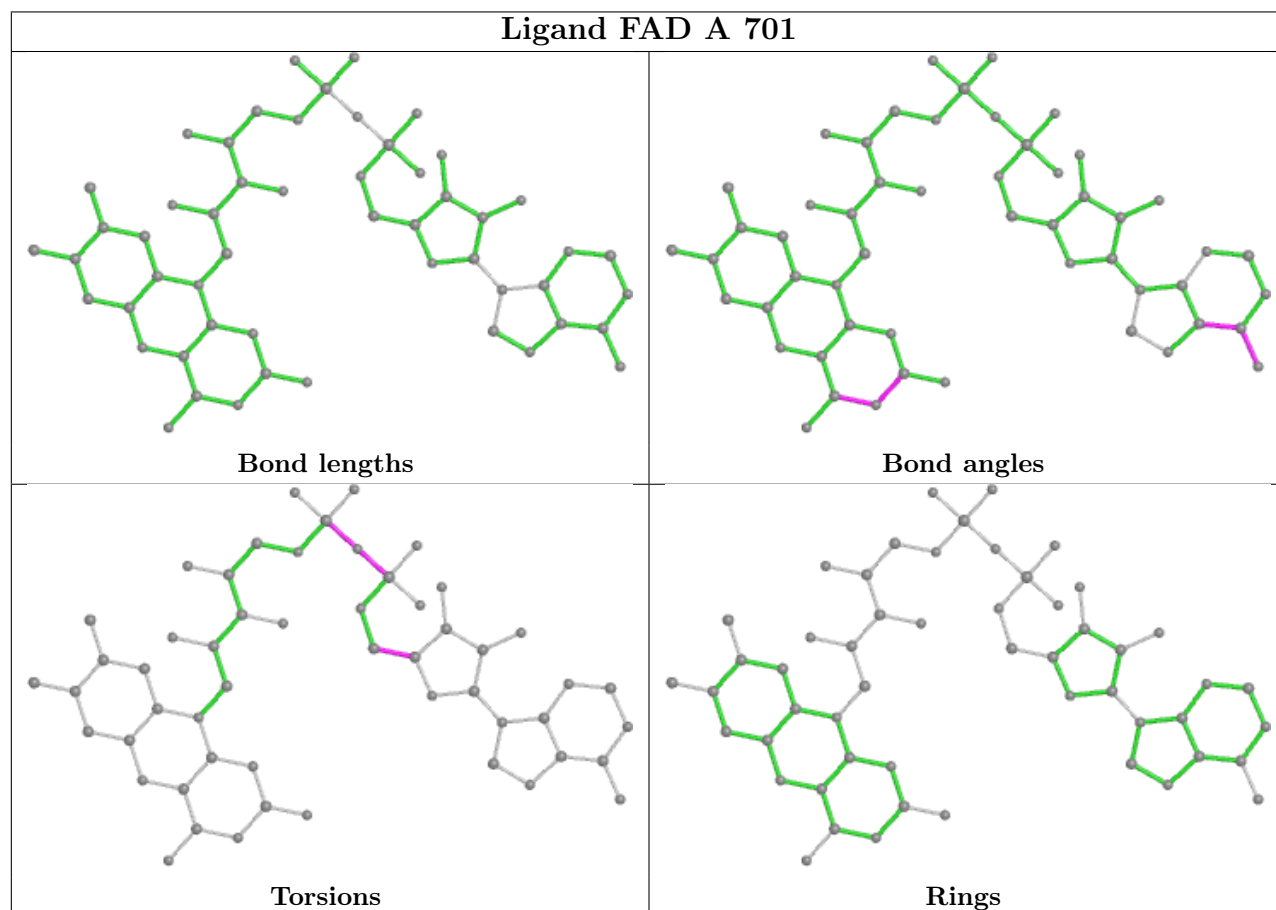
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 F3S A 702



Ligand FAD A 701



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	530/539 (98%)	-0.03	14 (2%) 56 27	50, 74, 93, 104	0
2	B	121/482 (25%)	0.41	14 (11%) 4 1	72, 97, 128, 144	0
3	C	117/121 (96%)	-0.15	1 (0%) 84 63	58, 83, 108, 121	0
All	All	768/1142 (67%)	0.02	29 (3%) 40 16	50, 78, 105, 144	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	422	ALA	5.0
1	A	446	ALA	4.1
2	B	420	ASP	3.9
2	B	424	LEU	3.9
2	B	358	THR	3.7

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](#)

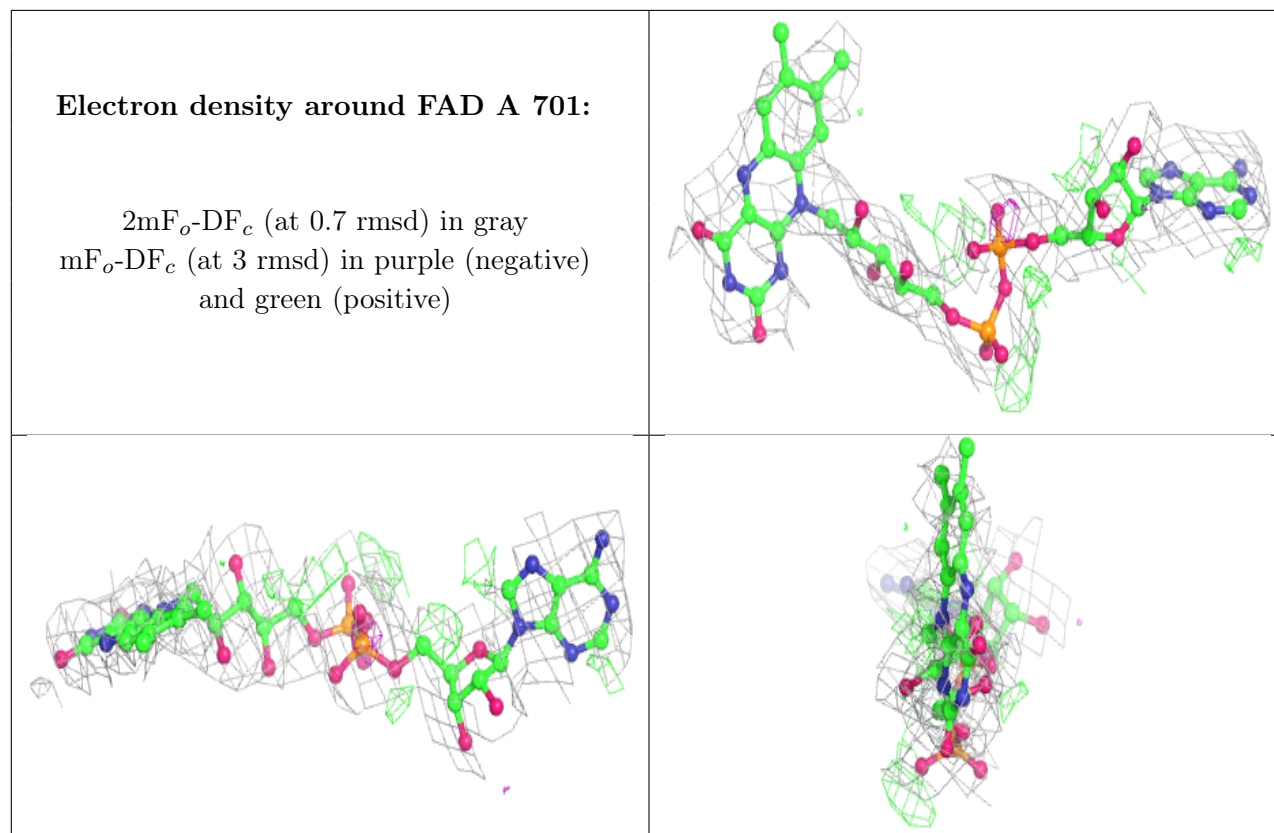
There are no monosaccharides in this entry.

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.

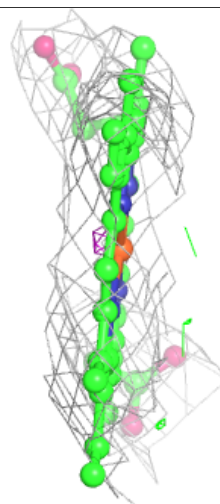
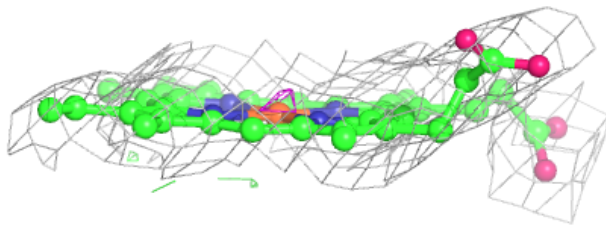
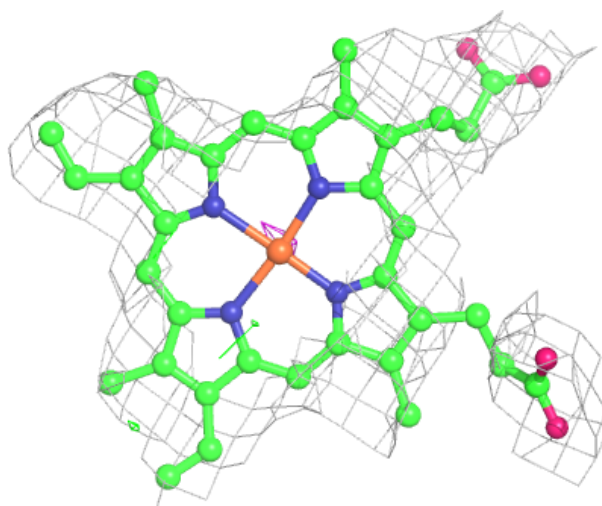
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	FAD	A	701	53/53	0.92	0.20	58,78,90,91	0
6	HEM	B	501	43/43	0.94	0.21	65,76,79,80	0
5	F3S	A	702	7/7	0.97	0.16	57,64,69,72	0

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.



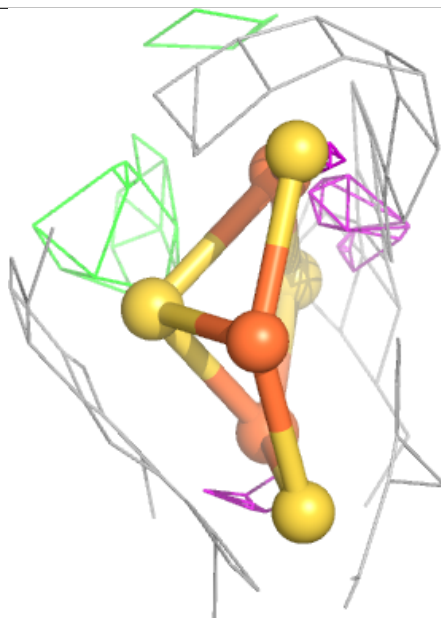
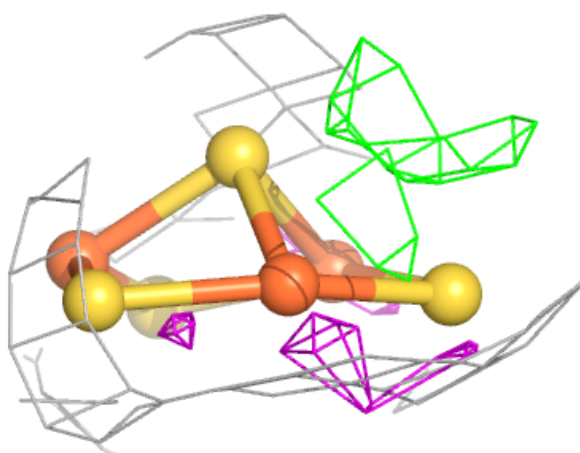
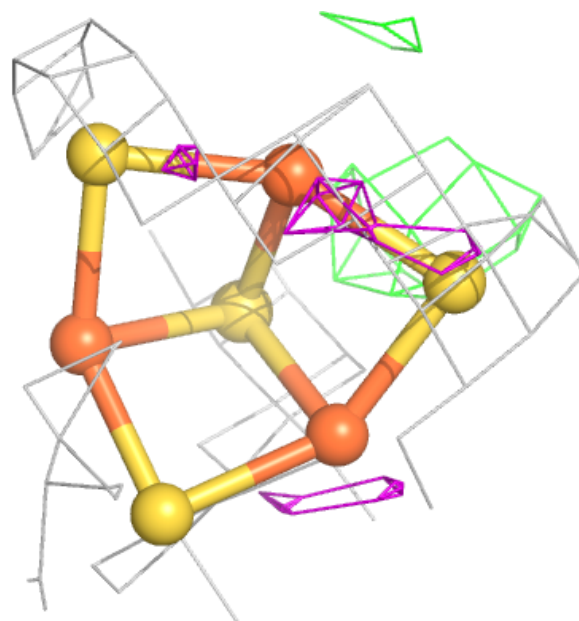
Electron density around HEM B 501:

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



Electron density around F3S A 702:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.