



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:08 AM UTC

PDB ID : 1DIQ / pdb_00001diq
Title : CRYSTAL STRUCTURE OF P-CRESOL METHYLHYDROXYLASE WITH
SUBSTRATE BOUND
Authors : Cunane, L.M.; Chen, Z.W.; Shamala, N.; Mathews, F.S.; Cronin, C.S.; McIn-
tire, W.S.
Deposited on : 1999-11-29
Resolution : 2.75 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

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

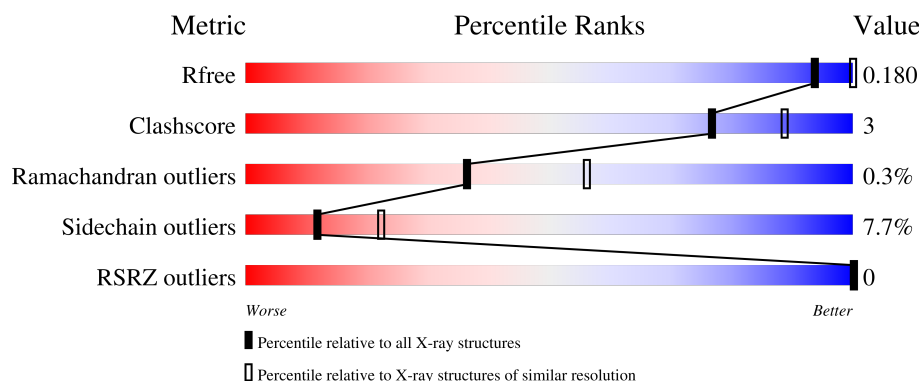
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	521	
1	B	521	
2	C	80	
2	D	80	

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
4	FAD	A	599	X	-	-	-
4	FAD	B	599	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9730 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 P-CRESOL METHYLHYDROXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	0	0	0
			4025	2562	688	748	27			
1	B	515	Total	C	N	O	S	0	0	0
			4025	2562	688	748	27			

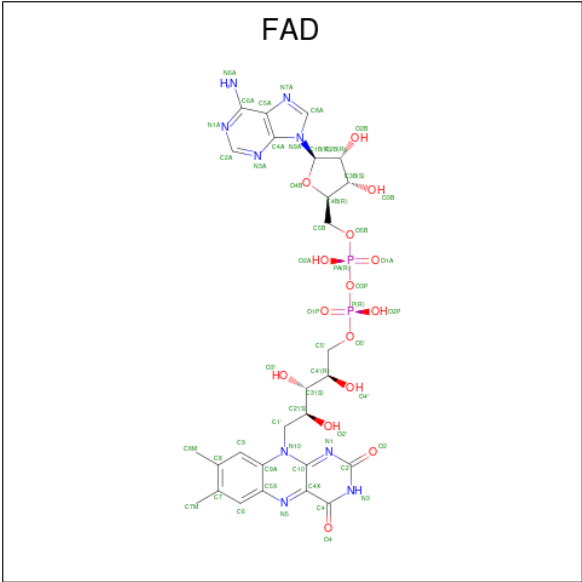
- Molecule 2 is a protein called P-CRESOL METHYLHYDROXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	74	Total	C	N	O	S	0	0	0
			564	358	96	107	3			
2	D	74	Total	C	N	O	S	0	0	0
			564	358	96	107	3			

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

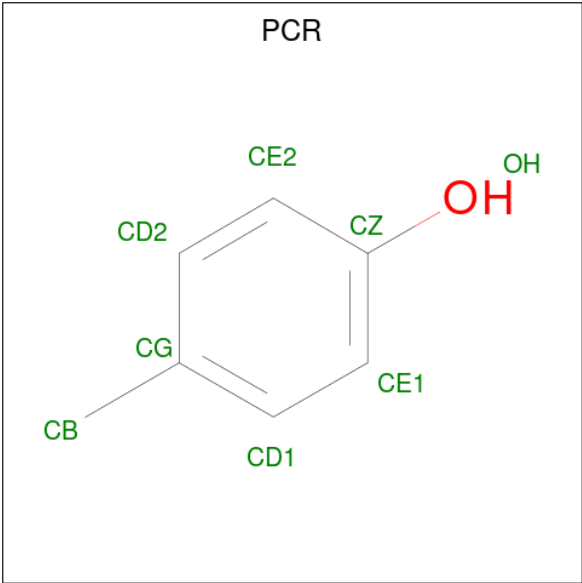
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



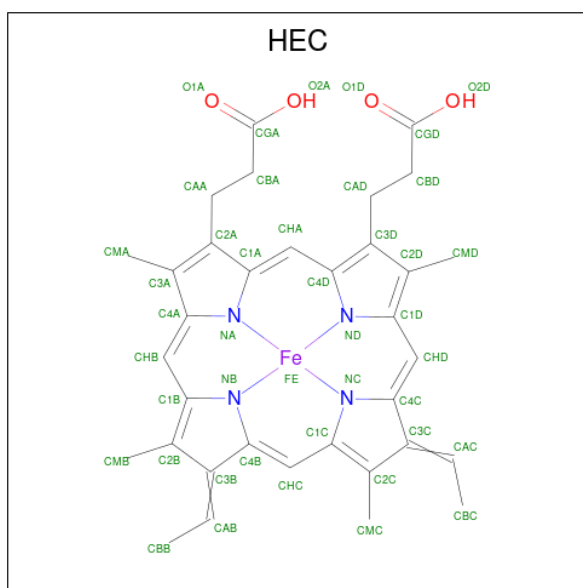
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0
			53	27	9	15	2	
4	B	1	Total	C	N	O	P	0
			53	27	9	15	2	

- Molecule 5 is P-CRESOL (CCD ID: PCR) (formula: C₇H₈O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	7	1		
5	B	1	Total	C	O	0	0
			8	7	1		

- Molecule 6 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



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

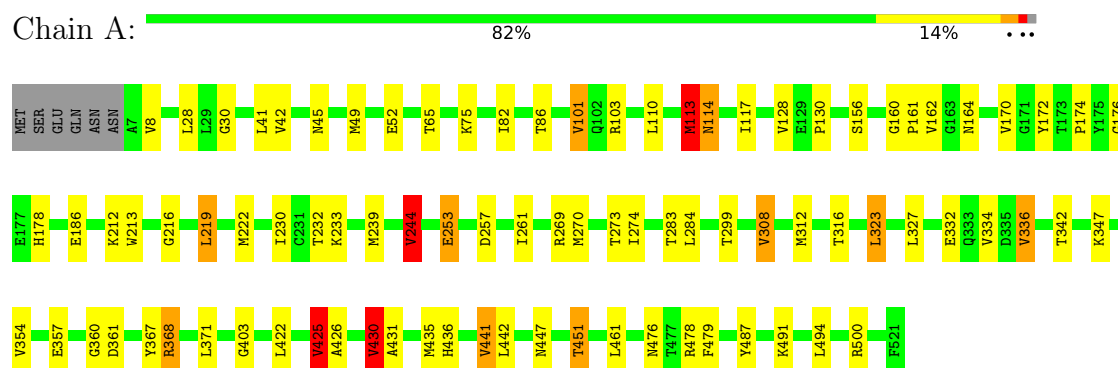
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	157	Total O 157 157	0	0
7	C	19	Total O 19 19	0	0
7	B	153	Total O 153 153	0	0
7	D	13	Total O 13 13	0	0

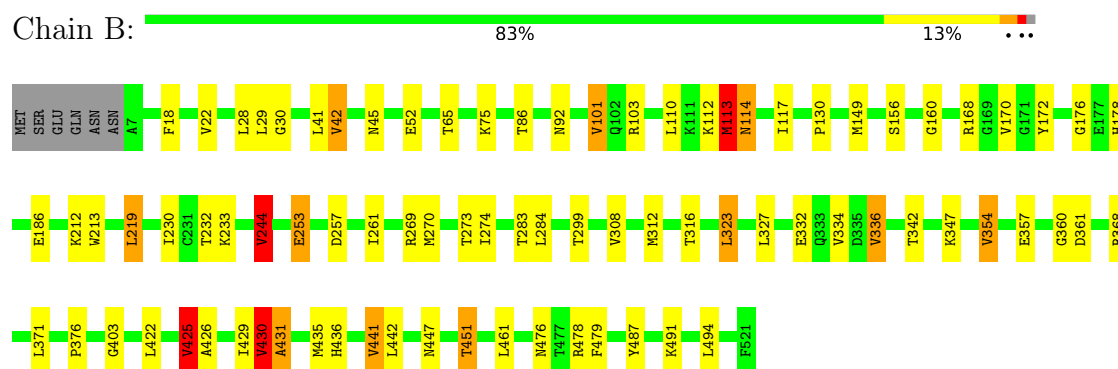
3 Residue-property plots [i](#)

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.

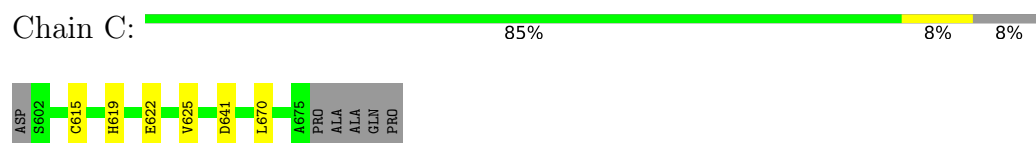
• Molecule 1: P-CRESOL METHYLHYDROXYLASE



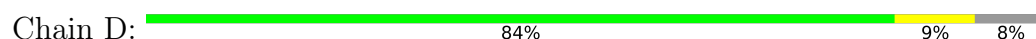
• Molecule 1: P-CRESOL METHYLHYDROXYLASE



• Molecule 2: P-CRESOL METHYLHYDROXYLASE



• Molecule 2: P-CRESOL METHYLHYDROXYLASE



ASP	S602	C615	H619	E622	V625	V643	E661	L670	A675	PRO	ALA	ALA	GLN	PRO
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	139.10Å 130.50Å 74.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.75 25.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	80.5 (25.00-2.75) 80.7 (25.00-2.75)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.49 (at 2.73Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.133 , 0.183 0.134 , 0.180	Depositor DCC
R_{free} test set	2913 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9730	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.77% 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: HEC, FAD, PCR, CL

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	0.81	8/4123 (0.2%)	1.20	22/5593 (0.4%)
1	B	0.81	9/4123 (0.2%)	1.20	22/5593 (0.4%)
2	C	0.83	2/579 (0.3%)	1.32	7/786 (0.9%)
2	D	0.86	2/579 (0.3%)	1.31	7/786 (0.9%)
All	All	0.82	21/9404 (0.2%)	1.22	58/12758 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	619	HIS	CE1-NE2	9.87	1.42	1.32
2	C	619	HIS	CE1-NE2	7.75	1.40	1.32
1	B	113	MET	SD-CE	-7.44	1.60	1.79
1	A	222	MET	SD-CE	-5.78	1.65	1.79
1	A	82	ILE	CA-CB	5.67	1.59	1.53
2	D	619	HIS	ND1-CE1	5.63	1.38	1.32
1	A	113	MET	SD-CE	-5.50	1.65	1.79
1	A	244	VAL	CA-CB	5.49	1.62	1.54
1	B	441	VAL	CA-CB	5.46	1.59	1.53
1	B	354	VAL	CA-CB	5.40	1.61	1.54
1	B	274	ILE	CA-C	5.31	1.57	1.53
2	C	619	HIS	ND1-CE1	5.29	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	308	VAL	CA-CB	5.29	1.60	1.54
1	B	42	VAL	CA-CB	5.28	1.60	1.54
1	A	425	VAL	CA-CB	5.27	1.60	1.53
1	A	49	MET	SD-CE	-5.20	1.66	1.79
1	B	244	VAL	CA-CB	5.17	1.62	1.54
1	B	270	MET	SD-CE	-5.12	1.66	1.79
1	A	270	MET	SD-CE	-5.11	1.66	1.79
1	B	425	VAL	CA-CB	5.06	1.60	1.53
1	B	149	MET	SD-CE	-5.00	1.67	1.79

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	619	HIS	ND1-CG-CD2	13.75	119.85	106.10
2	C	619	HIS	ND1-CG-CD2	13.69	119.79	106.10
1	A	213	TRP	N-CA-C	10.67	122.67	111.14
1	B	213	TRP	N-CA-C	10.53	122.51	111.14
1	A	219	LEU	N-CA-C	9.77	125.28	113.16
1	B	219	LEU	N-CA-C	9.55	125.00	113.16
1	A	430	VAL	N-CA-C	9.55	122.01	108.36
1	B	430	VAL	N-CA-C	9.40	121.80	108.36
2	D	619	HIS	CB-CG-CD2	-8.76	119.81	131.20
1	B	274	ILE	N-CA-C	-8.62	99.02	107.55
1	B	212	LYS	N-CA-C	8.56	120.30	110.97
2	C	619	HIS	CB-CG-CD2	-8.51	120.14	131.20
1	A	212	LYS	N-CA-C	8.29	120.01	110.97
1	B	403	GLY	N-CA-C	8.17	122.79	112.83
1	A	403	GLY	N-CA-C	7.92	122.49	112.83
1	A	253	GLU	N-CA-C	7.79	121.27	111.69
1	B	253	GLU	N-CA-C	7.73	121.20	111.69
2	C	619	HIS	N-CA-C	7.52	122.56	113.23
2	D	619	HIS	N-CA-C	7.50	122.53	113.23
1	B	178	HIS	N-CA-C	7.21	120.05	111.33
1	A	178	HIS	N-CA-C	7.10	119.92	111.33
1	A	101	VAL	CB-CA-C	-6.96	102.75	112.14
1	B	101	VAL	CB-CA-C	-6.65	103.16	112.14
1	A	176	GLY	N-CA-C	6.57	120.61	112.73
1	B	160	GLY	CA-C-N	6.47	125.70	118.97
1	B	160	GLY	C-N-CA	6.47	125.70	118.97
2	C	619	HIS	CG-CD2-NE2	-6.37	100.83	107.20
2	D	619	HIS	CG-CD2-NE2	-6.34	100.86	107.20
1	A	170	VAL	N-CA-C	6.25	117.48	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	GLY	N-CA-C	-6.21	105.71	112.04
1	B	30	GLY	N-CA-C	-6.01	105.91	112.04
1	B	426	ALA	N-CA-C	6.01	118.10	109.14
1	B	176	GLY	N-CA-C	5.82	119.71	112.73
2	C	615	CYS	N-CA-C	5.78	117.25	111.07
2	C	625	VAL	N-CA-C	-5.78	104.70	111.00
1	B	436	HIS	N-CA-C	-5.70	97.14	107.75
2	D	625	VAL	N-CA-C	-5.70	104.79	111.00
1	A	441	VAL	CB-CA-C	5.69	117.83	111.80
1	B	117	ILE	N-CA-C	5.68	116.46	110.72
2	C	619	HIS	CG-ND1-CE1	-5.55	99.87	109.30
1	A	160	GLY	CA-C-N	5.47	124.66	118.97
1	A	160	GLY	C-N-CA	5.47	124.66	118.97
2	D	619	HIS	CG-ND1-CE1	-5.41	100.11	109.30
1	A	426	ALA	N-CA-C	5.40	117.19	109.14
1	A	436	HIS	N-CA-C	-5.39	97.72	107.75
1	A	162	VAL	N-CA-C	5.38	115.58	110.42
1	A	117	ILE	N-CA-C	5.38	116.15	110.72
2	D	615	CYS	N-CA-C	5.32	117.49	111.11
1	B	431	ALA	N-CA-C	-5.21	102.46	110.58
1	B	273	THR	N-CA-C	-5.20	105.53	111.14
1	B	323	LEU	CA-CB-CG	5.19	134.45	116.30
1	A	128	VAL	N-CA-C	5.15	116.32	108.80
1	B	376	PRO	N-CA-C	5.15	119.17	111.14
1	B	29	LEU	N-CA-C	5.14	119.69	113.41
1	A	323	LEU	CA-CB-CG	5.12	134.21	116.30
1	B	170	VAL	N-CA-C	5.11	116.72	108.85
1	A	273	THR	N-CA-C	-5.08	105.63	111.07
1	A	274	ILE	N-CA-C	-5.08	97.90	108.88

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	172	TYR	Sidechain
1	B	172	TYR	Sidechain

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	4025	0	3959	27	0
1	B	4025	0	3959	23	0
2	C	564	0	543	1	0
2	D	564	0	543	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	53	0	29	3	0
4	B	53	0	30	2	0
5	A	8	0	8	1	0
5	B	8	0	8	1	0
6	C	43	0	30	0	0
6	D	43	0	30	1	0
7	A	157	0	0	4	0
7	B	153	0	0	2	0
7	C	19	0	0	1	0
7	D	13	0	0	1	0
All	All	9730	0	9139	54	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 (54) 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:312:MET:O	1:A:316:THR:HG22	1.80	0.81
1:B:312:MET:O	1:B:316:THR:HG22	1.81	0.81
1:A:114:ASN:HD22	1:A:114:ASN:H	1.36	0.74
1:B:114:ASN:H	1:B:114:ASN:HD22	1.34	0.72
1:B:476:ASN:HD21	1:B:479:PHE:HD2	1.44	0.65
1:A:476:ASN:HD21	1:A:479:PHE:HD2	1.46	0.62
1:A:368:ARG:NH2	7:A:816:HOH:O	2.43	0.52
2:D:661:GLU:HB2	7:D:234:HOH:O	2.10	0.51
1:B:110:LEU:HD22	1:B:113:MET:HE3	1.93	0.51
1:B:92:ASN:HA	4:B:599:FAD:H5'2	1.92	0.50
1:A:86:THR:HG21	1:A:230:ILE:HG23	1.92	0.50
1:A:130:PRO:HD3	1:A:232:THR:O	2.12	0.49
1:A:174:PRO:HD2	1:A:239:MET:SD	2.53	0.49
1:B:86:THR:HG21	1:B:230:ILE:HG23	1.93	0.49
1:A:244:VAL:HG22	1:A:334:VAL:HG21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:VAL:HG11	1:A:442:LEU:HD12	1.95	0.49
1:B:487:TYR:HB3	1:B:491:LYS:HD3	1.95	0.48
1:A:476:ASN:HD22	1:A:478:ARG:H	1.62	0.48
1:B:244:VAL:HG22	1:B:334:VAL:HG21	1.95	0.48
4:B:599:FAD:N1	4:B:599:FAD:O3'	2.34	0.48
1:A:110:LEU:HD22	1:A:113:MET:HE3	1.95	0.47
1:A:487:TYR:HB3	1:A:491:LYS:HD3	1.95	0.47
1:B:257:ASP:O	1:B:261:ILE:HG13	2.14	0.47
1:A:186:GLU:HB3	1:A:233:LYS:HB2	1.96	0.47
1:A:216:GLY:O	1:B:168:ARG:NH2	2.28	0.47
1:B:425:VAL:HG11	1:B:442:LEU:HD12	1.97	0.46
1:B:186:GLU:HB3	1:B:233:LYS:HB2	1.97	0.46
1:A:161:PRO:HD2	7:A:889:HOH:O	2.15	0.46
1:B:130:PRO:HD3	1:B:232:THR:O	2.16	0.46
1:A:114:ASN:HD22	1:A:114:ASN:N	2.06	0.45
1:B:476:ASN:HD22	1:B:478:ARG:H	1.64	0.45
1:B:269:ARG:HH21	1:B:431:ALA:HA	1.82	0.45
1:B:476:ASN:ND2	1:B:478:ARG:HB3	2.32	0.45
1:A:8:VAL:HG11	7:A:940:HOH:O	2.16	0.45
1:B:430:VAL:HB	1:B:435:MET:SD	2.57	0.45
2:C:641:ASP:HB3	7:C:193:HOH:O	2.16	0.44
1:A:269:ARG:HH21	1:A:431:ALA:HA	1.82	0.44
1:B:112:LYS:HB2	7:B:899:HOH:O	2.18	0.44
1:A:491:LYS:HE3	7:B:901:HOH:O	2.17	0.44
1:B:447:ASN:O	1:B:451:THR:HG23	2.18	0.44
1:A:164:ASN:HD22	4:A:599:FAD:H4'	1.83	0.43
1:A:336:VAL:HG11	1:B:336:VAL:HG11	1.99	0.43
1:A:476:ASN:ND2	1:A:478:ARG:HB3	2.33	0.43
1:A:430:VAL:HB	1:A:435:MET:SD	2.59	0.42
1:A:257:ASP:O	1:A:261:ILE:HG13	2.20	0.42
1:A:447:ASN:O	1:A:451:THR:HG23	2.19	0.42
2:D:643:VAL:HG21	6:D:699:HEC:HMB2	2.02	0.42
4:A:599:FAD:N1	4:A:599:FAD:O3'	2.36	0.41
4:A:599:FAD:N5	5:A:798:PCR:HB2	2.36	0.41
1:B:429:ILE:HD11	5:B:799:PCR:HD11	2.02	0.41
1:A:332:GLU:O	1:A:336:VAL:HG13	2.20	0.41
1:B:332:GLU:O	1:B:336:VAL:HG13	2.20	0.41
1:A:500:ARG:HD3	7:A:905:HOH:O	2.20	0.41
1:B:18:PHE:O	1:B:22:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	513/521 (98%)	498 (97%)	13 (2%)	2 (0%)	30	50
1	B	513/521 (98%)	499 (97%)	12 (2%)	2 (0%)	30	50
2	C	72/80 (90%)	69 (96%)	3 (4%)	0	100	100
2	D	72/80 (90%)	69 (96%)	3 (4%)	0	100	100
All	All	1170/1202 (97%)	1135 (97%)	31 (3%)	4 (0%)	36	56

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	SER
1	B	156	SER
1	A	360	GLY
1	B	360	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	427/433 (99%)	391 (92%)	36 (8%)	10	19
1	B	427/433 (99%)	392 (92%)	35 (8%)	10	20
2	C	60/64 (94%)	58 (97%)	2 (3%)	33	57
2	D	60/64 (94%)	58 (97%)	2 (3%)	33	57
All	All	974/994 (98%)	899 (92%)	75 (8%)	12	22

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	41	LEU
1	A	42	VAL
1	A	45	ASN
1	A	52	GLU
1	A	65	THR
1	A	75	LYS
1	A	101	VAL
1	A	103	ARG
1	A	113	MET
1	A	114	ASN
1	A	219	LEU
1	A	244	VAL
1	A	253	GLU
1	A	283	THR
1	A	284	LEU
1	A	299	THR
1	A	308	VAL
1	A	323	LEU
1	A	327	LEU
1	A	336	VAL
1	A	342	THR
1	A	347	LYS
1	A	354	VAL
1	A	357	GLU
1	A	361	ASP
1	A	367	TYR
1	A	368	ARG
1	A	371	LEU
1	A	422	LEU
1	A	425	VAL
1	A	430	VAL
1	A	441	VAL
1	A	451	THR
1	A	461	LEU
1	A	494	LEU
2	C	622	GLU
2	C	670	LEU
1	B	28	LEU
1	B	41	LEU
1	B	42	VAL
1	B	45	ASN

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Mol	Chain	Res	Type
1	B	52	GLU
1	B	65	THR
1	B	75	LYS
1	B	101	VAL
1	B	103	ARG
1	B	113	MET
1	B	114	ASN
1	B	219	LEU
1	B	244	VAL
1	B	253	GLU
1	B	283	THR
1	B	284	LEU
1	B	299	THR
1	B	308	VAL
1	B	323	LEU
1	B	327	LEU
1	B	336	VAL
1	B	342	THR
1	B	347	LYS
1	B	354	VAL
1	B	357	GLU
1	B	361	ASP
1	B	368	ARG
1	B	371	LEU
1	B	422	LEU
1	B	425	VAL
1	B	430	VAL
1	B	441	VAL
1	B	451	THR
1	B	461	LEU
1	B	494	LEU
2	D	622	GLU
2	D	670	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	114	ASN
1	A	313	GLN
1	A	459	ASN
1	A	476	ASN

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Mol	Chain	Res	Type
1	A	519	ASN
1	B	40	GLN
1	B	114	ASN
1	B	313	GLN
1	B	459	ASN
1	B	476	ASN
1	B	519	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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	FAD	A	599	1	58,58,58	1.76	16 (27%)	85,89,89	1.74	17 (20%)
5	PCR	A	798	-	8,8,8	2.05	3 (37%)	10,10,10	0.33	0
5	PCR	B	799	-	8,8,8	1.84	2 (25%)	10,10,10	0.23	0
4	FAD	B	599	1	58,58,58	1.67	14 (24%)	85,89,89	1.75	17 (20%)
6	HEC	D	699	2	46,50,50	1.65	7 (15%)	58,82,82	1.43	3 (5%)
6	HEC	C	699	2	46,50,50	1.63	5 (10%)	58,82,82	1.47	3 (5%)

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
4	FAD	A	599	1	3/3/9/9	9/34/50/50	0/6/6/6
5	PCR	A	798	-	-	-	0/1/1/1
5	PCR	B	799	-	-	-	0/1/1/1
4	FAD	B	599	1	3/3/9/9	8/34/50/50	0/6/6/6
6	HEC	D	699	2	-	6/14/54/54	-
6	HEC	C	699	2	-	6/14/54/54	-

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	699	HEC	CAC-C3C	6.12	1.54	1.35
6	C	699	HEC	CAB-C3B	6.09	1.54	1.35
6	D	699	HEC	CAB-C3B	5.81	1.53	1.35
6	D	699	HEC	CAC-C3C	5.17	1.51	1.35
4	A	599	FAD	C4X-N5	4.32	1.40	1.30
4	B	599	FAD	C4X-N5	4.13	1.39	1.30
4	B	599	FAD	C10-N10	3.79	1.45	1.37
4	A	599	FAD	C8M-C8	-3.55	1.44	1.51
5	A	798	PCR	CE2-CD2	3.54	1.44	1.38
4	A	599	FAD	C1'-C2'	3.52	1.57	1.52
4	A	599	FAD	C10-N10	3.44	1.44	1.37
5	A	798	PCR	CE1-CD1	3.27	1.44	1.38
4	B	599	FAD	C6-C5X	3.20	1.44	1.40
4	B	599	FAD	C9-C8	-3.20	1.35	1.39
5	B	799	PCR	CE2-CD2	3.10	1.43	1.38
4	B	599	FAD	C8A-N7A	-3.07	1.25	1.31
4	A	599	FAD	P-O3P	-3.00	1.56	1.59
4	A	599	FAD	C5'-C4'	-2.94	1.47	1.51
5	B	799	PCR	CE1-CD1	2.93	1.43	1.38
4	A	599	FAD	C6-C5X	2.88	1.44	1.40
4	B	599	FAD	C1'-C2'	2.84	1.56	1.52
6	D	699	HEC	O1A-CGA	2.69	1.30	1.22
4	A	599	FAD	C4A-N3A	2.58	1.39	1.34
4	A	599	FAD	C9-C8	-2.53	1.36	1.39
4	A	599	FAD	O5'-C5'	-2.52	1.35	1.44
4	A	599	FAD	C8A-N7A	-2.52	1.26	1.31
4	B	599	FAD	O5'-C5'	-2.50	1.35	1.44
6	D	699	HEC	CMC-C2C	2.50	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	599	FAD	P-O3P	-2.49	1.56	1.59
4	B	599	FAD	C8M-C8	-2.44	1.46	1.51
4	A	599	FAD	C9A-N10	2.43	1.45	1.41
6	D	699	HEC	O2A-CGA	-2.43	1.22	1.30
6	D	699	HEC	CMD-C2D	2.29	1.55	1.50
4	B	599	FAD	C9A-N10	2.29	1.45	1.41
4	B	599	FAD	O4B-C1B	2.27	1.47	1.42
6	C	699	HEC	CMD-C2D	2.23	1.55	1.50
4	B	599	FAD	O2-C2	-2.21	1.20	1.24
4	A	599	FAD	C2B-C3B	-2.20	1.47	1.53
6	C	699	HEC	O1A-CGA	2.20	1.29	1.22
4	A	599	FAD	P-O2P	-2.18	1.45	1.55
4	A	599	FAD	C8A-N9A	2.14	1.41	1.37
4	B	599	FAD	C4A-N3A	2.12	1.38	1.34
6	C	699	HEC	CMC-C2C	2.11	1.55	1.50
6	D	699	HEC	C3C-C2C	-2.08	1.34	1.41
5	A	798	PCR	CE2-CZ	2.04	1.42	1.39
4	B	599	FAD	P-O2P	-2.02	1.46	1.55
4	A	599	FAD	C10-N1	2.01	1.37	1.33

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	699	HEC	CBB-CAB-C3B	-6.83	113.78	127.43
6	D	699	HEC	CBB-CAB-C3B	-6.75	113.94	127.43
6	C	699	HEC	CBC-CAC-C3C	-6.04	115.36	127.43
6	D	699	HEC	CBC-CAC-C3C	-5.99	115.46	127.43
4	B	599	FAD	C5'-C4'-C3'	-5.49	101.86	112.22
4	A	599	FAD	O4'-C4'-C3'	5.47	122.05	109.25
4	A	599	FAD	C5'-C4'-C3'	-5.30	102.21	112.22
4	B	599	FAD	O3'-C3'-C4'	-5.14	97.26	108.93
4	B	599	FAD	O4'-C4'-C3'	5.01	120.97	109.25
4	B	599	FAD	O4'-C4'-C5'	4.79	120.56	109.99
4	A	599	FAD	O3'-C3'-C4'	-4.44	98.85	108.93
4	A	599	FAD	C4'-C3'-C2'	4.18	120.53	113.57
4	B	599	FAD	C4'-C3'-C2'	3.94	120.12	113.57
4	B	599	FAD	C4A-N9A-C8A	-3.88	101.67	105.74
4	A	599	FAD	C4A-N9A-C8A	-3.84	101.70	105.74
4	A	599	FAD	O4'-C4'-C5'	3.58	117.87	109.99
4	B	599	FAD	C5X-N5-C4X	-3.07	113.12	118.09
4	B	599	FAD	C9A-C5X-N5	3.04	125.69	122.45
4	A	599	FAD	N3-C2-N1	-3.01	113.11	119.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	599	FAD	C5X-N5-C4X	-2.96	113.31	118.09
4	A	599	FAD	C9A-C5X-N5	2.90	125.53	122.45
4	B	599	FAD	C1B-N9A-C8A	-2.86	120.74	127.09
4	B	599	FAD	C2B-C1B-N9A	-2.86	106.20	113.30
4	A	599	FAD	O4B-C1B-N9A	2.78	113.42	108.09
4	A	599	FAD	C2B-C1B-N9A	-2.72	106.55	113.30
4	A	599	FAD	C10-N1-C2	2.65	122.59	116.85
4	A	599	FAD	C1B-N9A-C8A	-2.64	121.23	127.09
4	B	599	FAD	O4B-C1B-N9A	2.58	113.05	108.09
4	B	599	FAD	O3'-C3'-C2'	2.58	114.78	108.93
4	B	599	FAD	C10-N1-C2	2.55	122.36	116.85
4	A	599	FAD	O3'-C3'-C2'	2.43	114.45	108.93
6	C	699	HEC	O1A-CGA-CBA	-2.41	115.43	123.09
4	A	599	FAD	O2-C2-N3	2.37	123.14	118.58
4	A	599	FAD	O2'-C2'-C3'	2.36	114.76	109.25
4	B	599	FAD	N3-C2-N1	-2.35	114.50	119.50
4	B	599	FAD	O2-C2-N3	2.34	123.08	118.58
6	D	699	HEC	O1A-CGA-CBA	-2.33	115.69	123.09
4	B	599	FAD	O2'-C2'-C3'	2.21	114.42	109.25
4	B	599	FAD	N9A-C8A-N7A	2.02	116.80	113.94
4	A	599	FAD	N9A-C8A-N7A	2.01	116.79	113.94

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	599	FAD	C2'
4	A	599	FAD	C3'
4	A	599	FAD	C4'
4	B	599	FAD	C2'
4	B	599	FAD	C3'
4	B	599	FAD	C4'

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	599	FAD	N10-C1'-C2'-O2'
4	A	599	FAD	N10-C1'-C2'-C3'
4	A	599	FAD	C2'-C3'-C4'-C5'
4	A	599	FAD	O3'-C3'-C4'-C5'
4	A	599	FAD	C3'-C4'-C5'-O5'
4	A	599	FAD	O4'-C4'-C5'-O5'
4	B	599	FAD	N10-C1'-C2'-O2'

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Mol	Chain	Res	Type	Atoms
4	B	599	FAD	N10-C1'-C2'-C3'
4	B	599	FAD	C3'-C4'-C5'-O5'
4	B	599	FAD	O4'-C4'-C5'-O5'
6	C	699	HEC	C2B-C3B-CAB-CBB
6	C	699	HEC	C4B-C3B-CAB-CBB
6	C	699	HEC	C2C-C3C-CAC-CBC
6	C	699	HEC	C4C-C3C-CAC-CBC
6	D	699	HEC	C2B-C3B-CAB-CBB
6	D	699	HEC	C4B-C3B-CAB-CBB
6	D	699	HEC	C2C-C3C-CAC-CBC
6	D	699	HEC	C4C-C3C-CAC-CBC
4	B	599	FAD	O3'-C3'-C4'-C5'
4	B	599	FAD	C2'-C3'-C4'-C5'
4	A	599	FAD	O3'-C3'-C4'-O4'
4	A	599	FAD	C2'-C3'-C4'-O4'
4	B	599	FAD	O3'-C3'-C4'-O4'
4	B	599	FAD	C4'-C5'-O5'-P
4	A	599	FAD	C4'-C5'-O5'-P
6	D	699	HEC	CAD-CBD-CGD-O1D
6	D	699	HEC	CAD-CBD-CGD-O2D
6	C	699	HEC	CAD-CBD-CGD-O2D
6	C	699	HEC	CAD-CBD-CGD-O1D

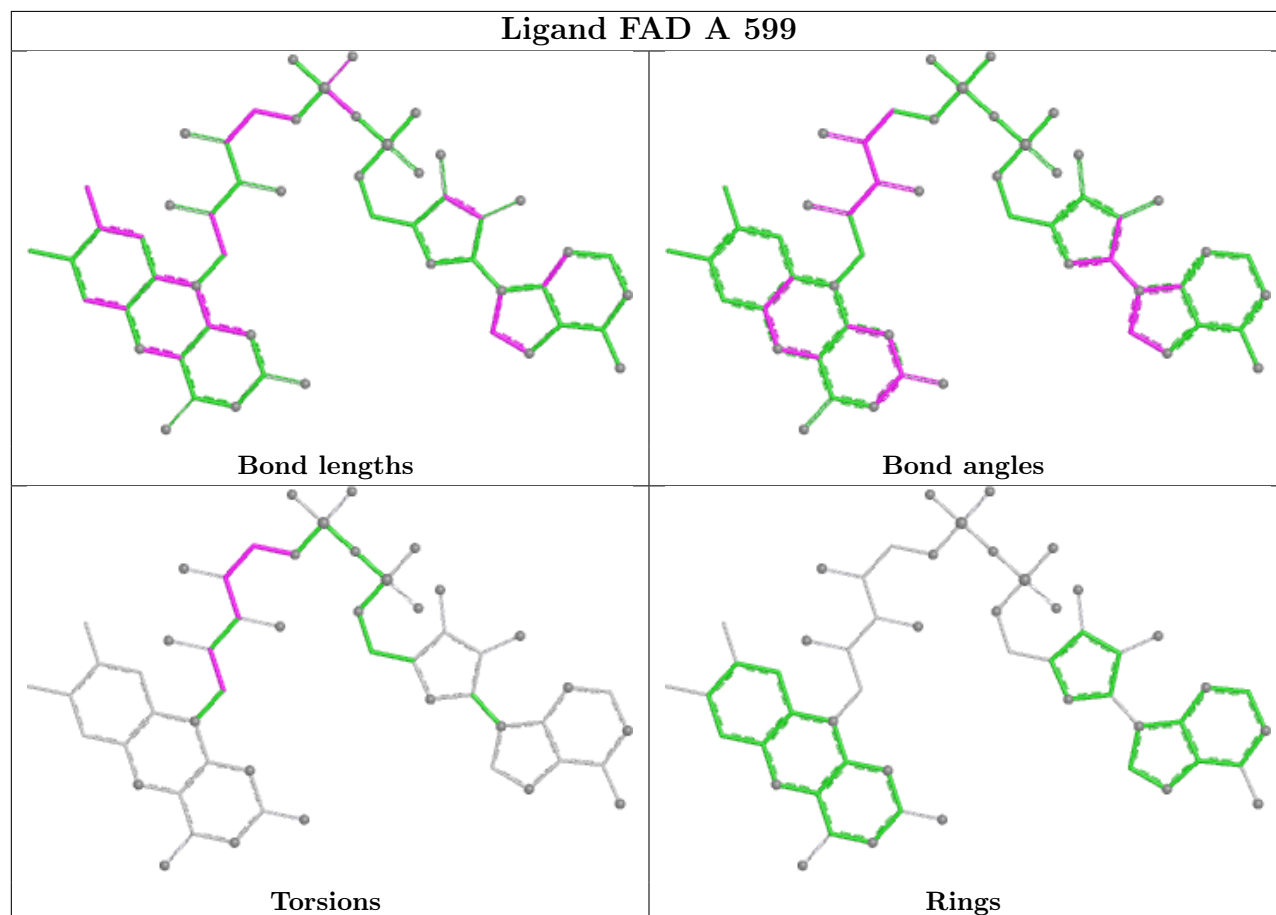
There are no ring outliers.

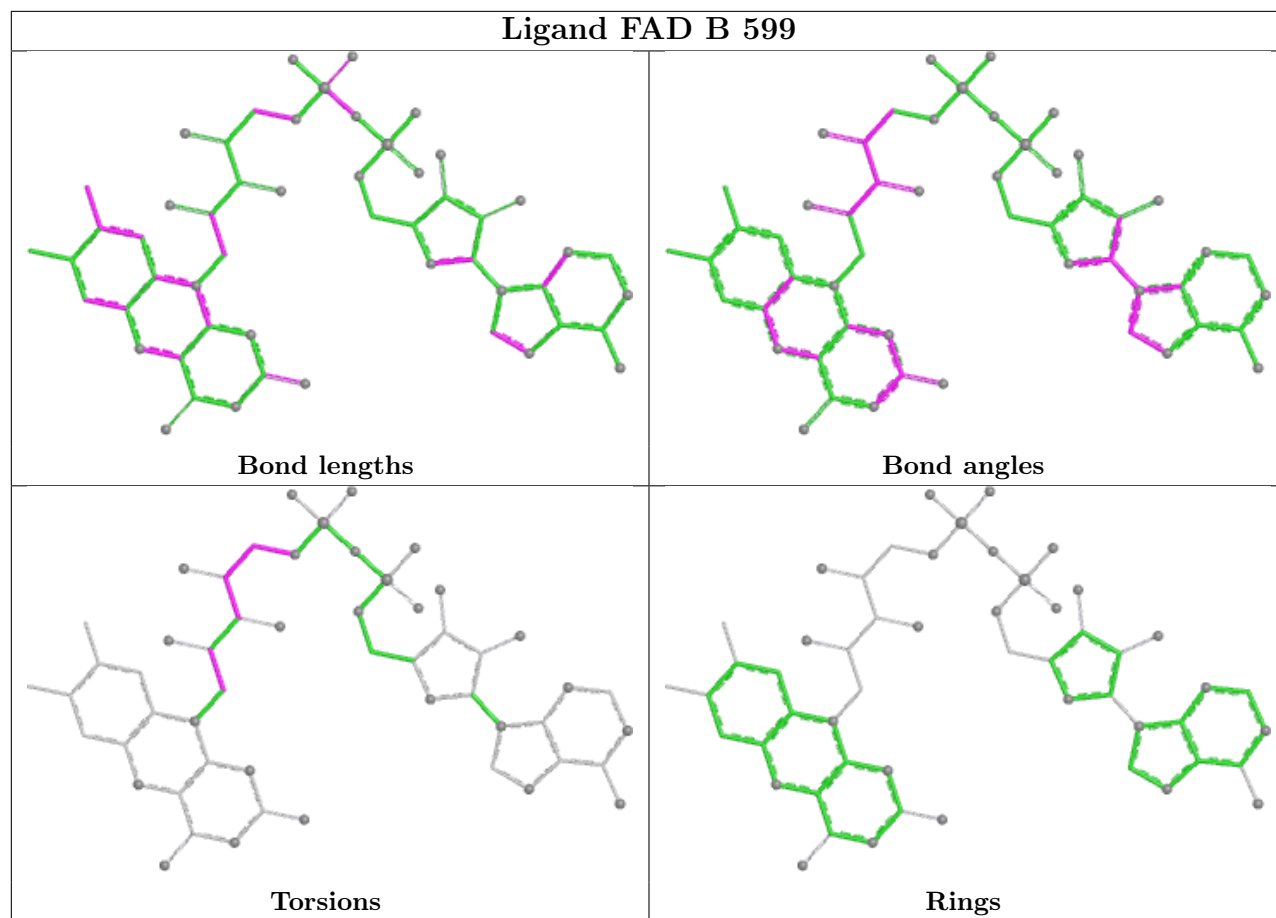
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	599	FAD	3	0
5	A	798	PCR	1	0
5	B	799	PCR	1	0
4	B	599	FAD	2	0
6	D	699	HEC	1	0

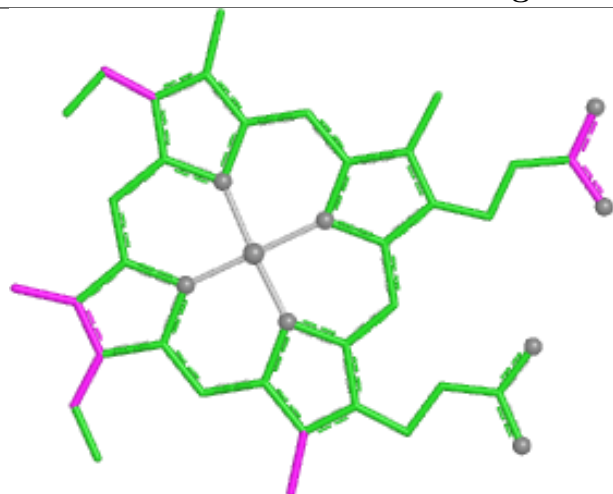
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

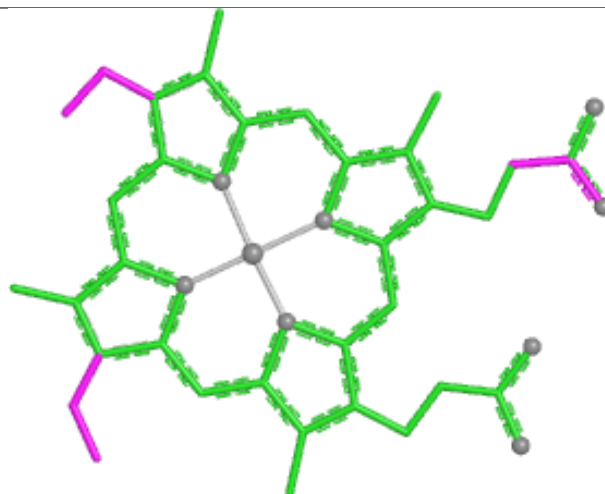




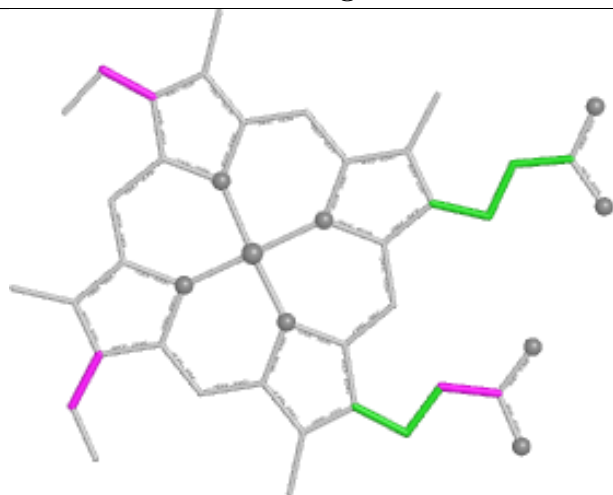
Ligand HEC D 699



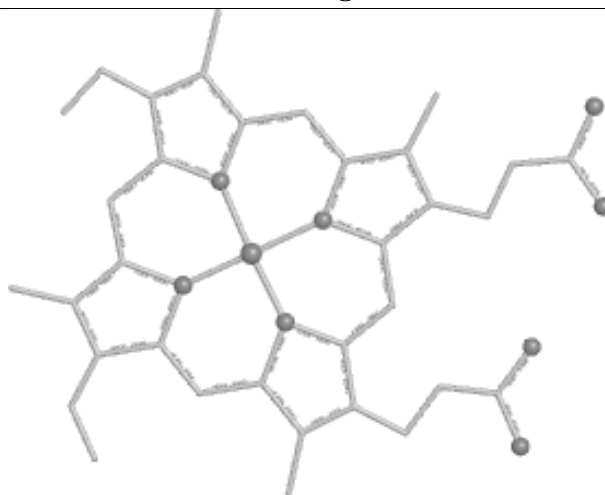
Bond lengths



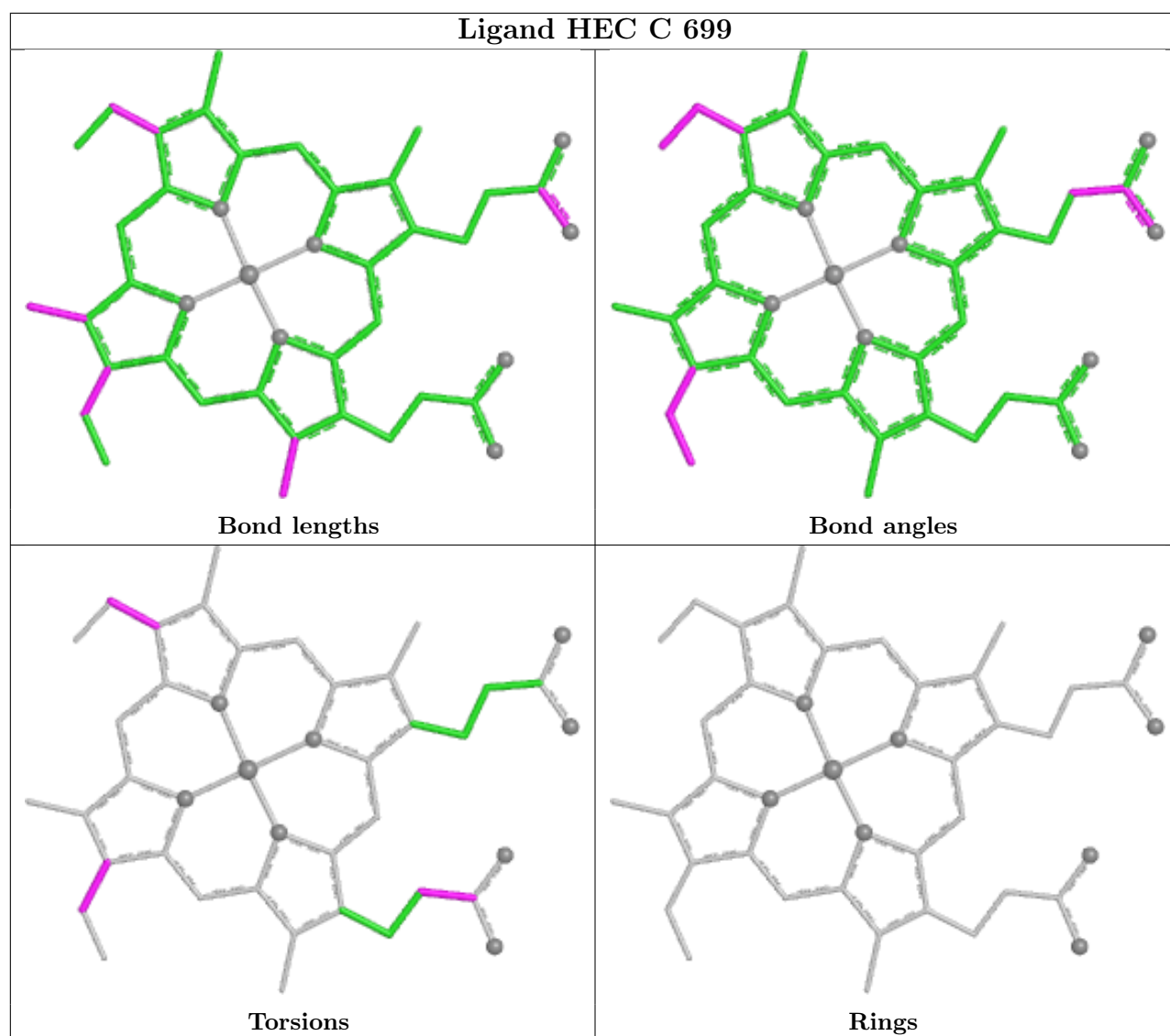
Bond angles



Torsions



Rings



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	515/521 (98%)	-1.30	0 100 100	17, 37, 73, 85	0
1	B	515/521 (98%)	-1.31	0 100 100	19, 37, 71, 84	0
2	C	74/80 (92%)	-1.16	0 100 100	26, 43, 76, 87	0
2	D	74/80 (92%)	-1.25	0 100 100	31, 47, 74, 87	0
All	All	1178/1202 (98%)	-1.30	0 100 100	17, 38, 73, 87	0

There are no RSRZ outliers to report.

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 oligosaccharides 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.

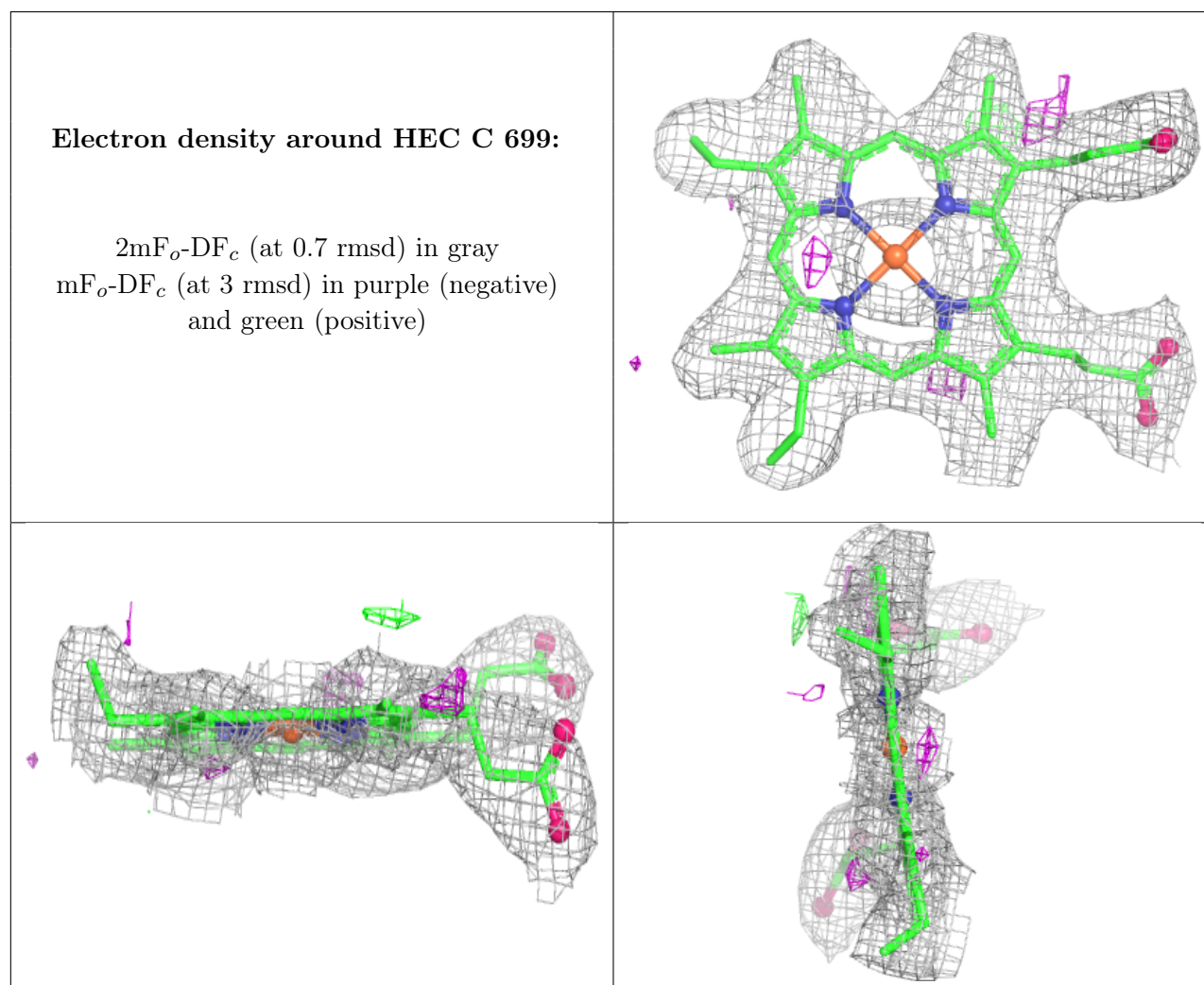
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PCR	B	799	8/8	0.97	0.05	25,28,33,34	0
6	HEC	C	699	43/43	0.97	0.05	25,37,48,59	0
6	HEC	D	699	43/43	0.97	0.05	23,40,51,55	0
5	PCR	A	798	8/8	0.98	0.04	13,25,31,32	0

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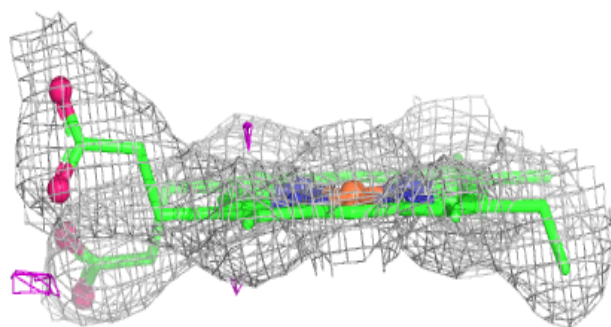
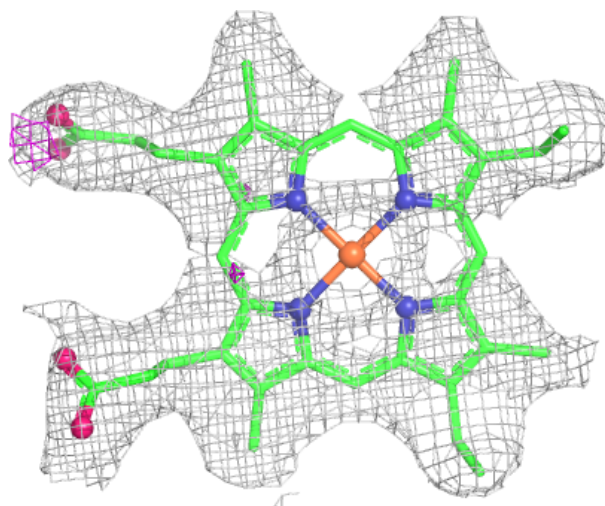
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	B	701	1/1	0.98	0.03	36,36,36,36	0
4	FAD	A	599	53/53	0.98	0.04	11,24,33,35	0
4	FAD	B	599	53/53	0.98	0.03	16,27,32,35	0
3	CL	A	702	1/1	0.99	0.01	39,39,39,39	0

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.



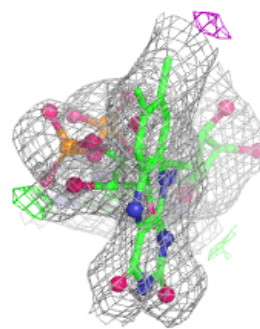
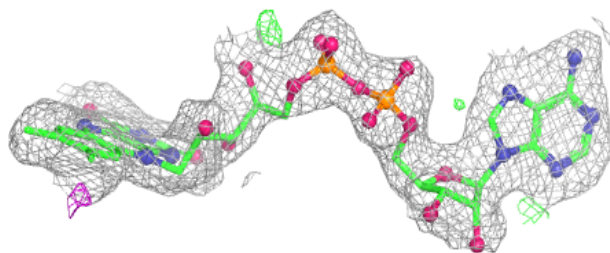
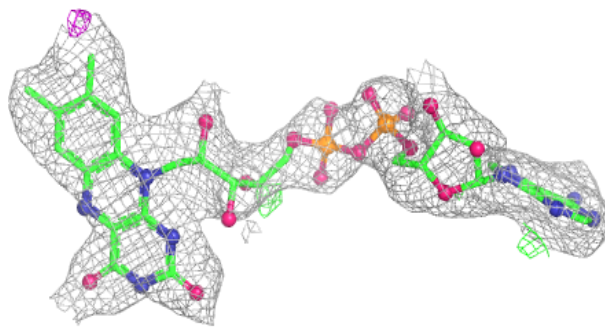
Electron density around HEC D 699:

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

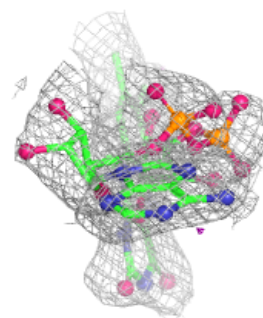
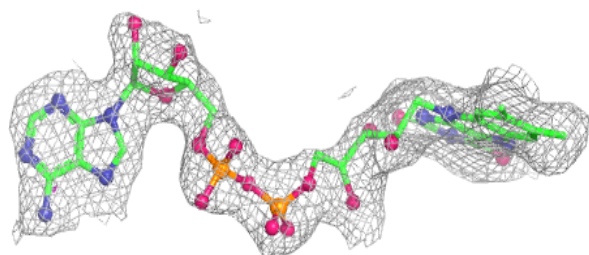
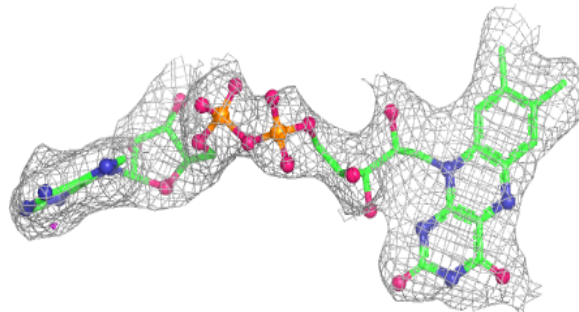


Electron density around FAD A 599:

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

**Electron density around FAD B 599:**

$2mF_o-DF_c$ (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.