



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:39 PM UTC

PDB ID : 3VRD / pdb_00003vrd
Title : Crystal structure of flavocytochrome c from *Thermochromatium tepidum*
Authors : Hirano, Y.; Kimura, Y.; Suzuki, H.; Miki, K.; Wang, Z.-Y.
Deposited on : 2012-04-09
Resolution : 1.50 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

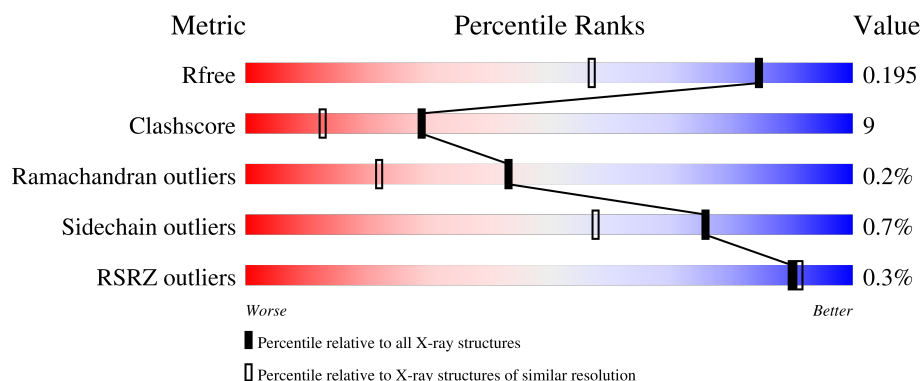
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	174	
2	B	401	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5107 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.

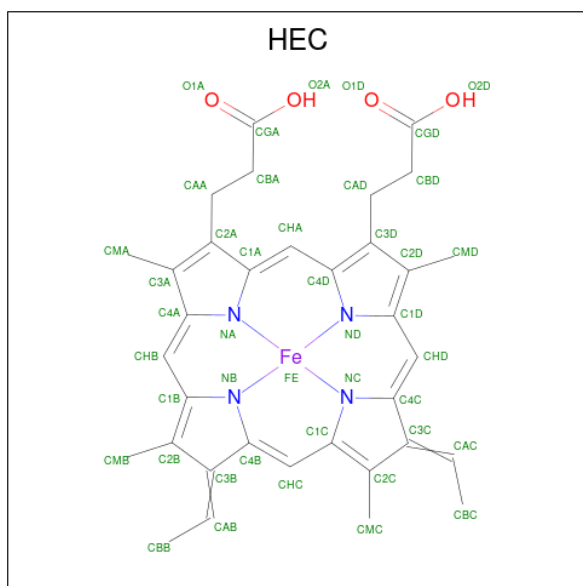
- Molecule 1 is a protein called Flavocytochrome c heme subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	1	0
			1370	863	233	263	11			

- Molecule 2 is a protein called Flavocytochrome c flavin subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	400	Total	C	N	O	S	0	0	0
			3015	1912	512	579	12			

- Molecule 3 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



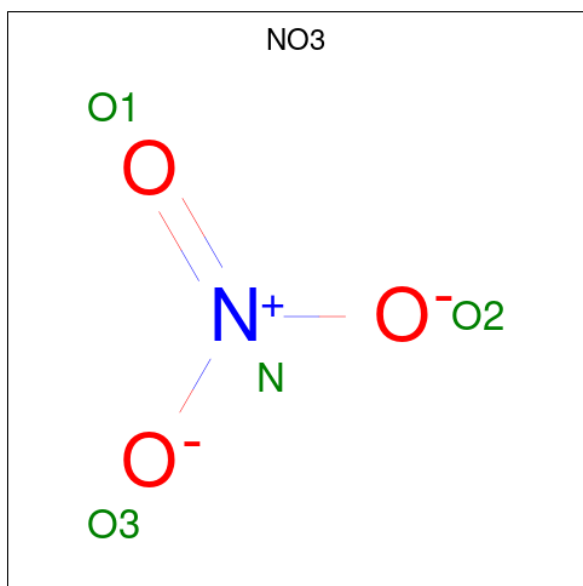
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	1
			47	36	1	4	6		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



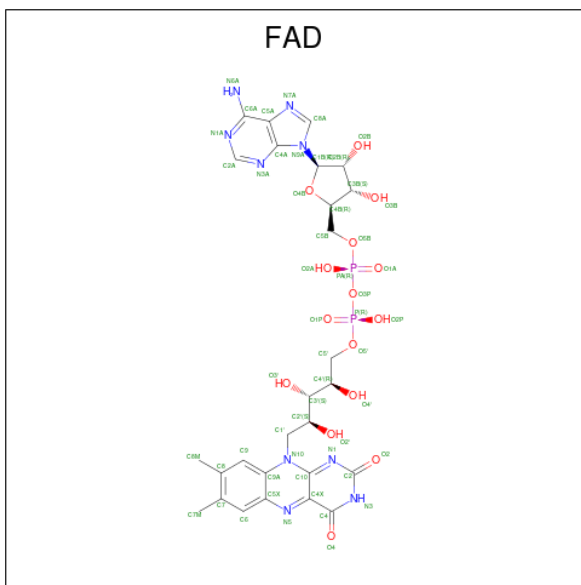
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is NITRATE ION (CCD ID: NO3) (formula: NO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 4	N 1	O 3	0	0
5	B	1	Total 4	N 1	O 3	0	0

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



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

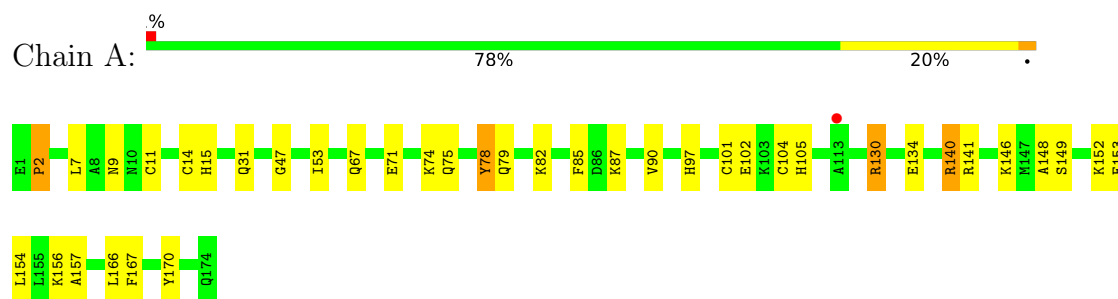
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	186	Total O 186 186	0	0
7	B	367	Total O 367 367	0	0

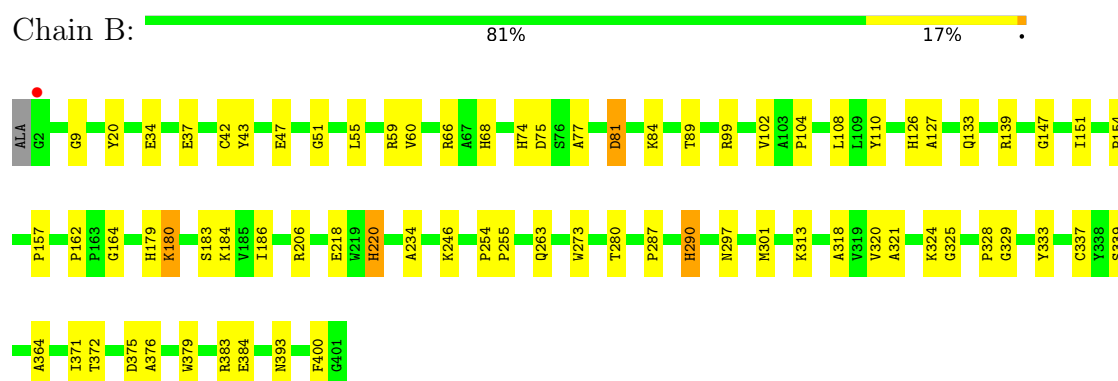
3 Residue-property plots

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: Flavocytochrome c heme subunit



- Molecule 2: Flavocytochrome c flavin subunit



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	140.62Å 140.62Å 57.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.50 50.00 – 1.50	Depositor EDS
% Data completeness (in resolution range)	93.3 (50.00-1.50) 93.3 (50.00-1.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.67 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.160 , 0.195 0.160 , 0.195	Depositor DCC
R_{free} test set	4208 reflections (0.71%)	wwPDB-VP
Wilson B-factor (Å ²)	8.5	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.037 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5107	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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: GOL, CSS, HEC, FAD, NO3

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	1.70	12/1402 (0.9%)	1.66	8/1881 (0.4%)
2	B	1.80	35/3073 (1.1%)	1.48	8/4184 (0.2%)
All	All	1.77	47/4475 (1.1%)	1.54	16/6065 (0.3%)

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	290	HIS	ND1-CE1	8.33	1.40	1.32
2	B	329	GLY	N-CA	7.67	1.55	1.45
1	A	134	GLU	N-CA	7.64	1.55	1.46
2	B	220	HIS	ND1-CE1	7.41	1.40	1.32
2	B	59	ARG	N-CA	7.06	1.54	1.46
2	B	339	SER	N-CA	6.94	1.54	1.46
2	B	47	GLU	N-CA	6.74	1.54	1.46
2	B	139	ARG	N-CA	6.38	1.54	1.46
2	B	301	MET	N-CA	6.32	1.54	1.45
2	B	68	HIS	ND1-CE1	6.18	1.38	1.32
2	B	51	GLY	N-CA	6.08	1.53	1.45
2	B	164	GLY	C-O	-6.06	1.18	1.24
2	B	183	SER	C-O	-5.98	1.16	1.23
2	B	206	ARG	CA-C	-5.96	1.44	1.52
2	B	318	ALA	C-O	5.90	1.31	1.24
1	A	130	ARG	N-CA	5.85	1.53	1.46
2	B	328	PRO	C-O	5.79	1.30	1.23
1	A	15	HIS	CE1-NE2	5.79	1.38	1.32
1	A	140	ARG	CD-NE	-5.77	1.38	1.46
2	B	383	ARG	CZ-NH2	5.77	1.41	1.33
1	A	130	ARG	CZ-NH2	-5.74	1.25	1.33
1	A	78	TYR	C-O	5.67	1.30	1.23
1	A	79	GLN	CA-C	5.60	1.59	1.52
1	A	31	GLN	N-CA	5.54	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	89	THR	N-CA	5.52	1.52	1.45
2	B	320	VAL	C-O	5.48	1.30	1.24
2	B	9	GLY	N-CA	5.44	1.53	1.45
2	B	126	HIS	CE1-NE2	5.44	1.38	1.32
2	B	321	ALA	N-CA	5.42	1.52	1.46
2	B	325	GLY	N-CA	5.42	1.53	1.45
2	B	162	PRO	C-N	5.40	1.39	1.34
2	B	110	TYR	N-CA	5.39	1.52	1.46
2	B	55	LEU	N-CA	-5.38	1.39	1.46
2	B	255	PRO	CA-C	-5.36	1.46	1.52
1	A	2	PRO	C-O	5.34	1.29	1.23
2	B	287	PRO	N-CA	-5.33	1.40	1.47
2	B	77	ALA	C-O	5.32	1.30	1.24
2	B	375	ASP	C-O	5.30	1.30	1.23
2	B	164	GLY	N-CA	5.30	1.49	1.44
2	B	154	PRO	N-CA	5.30	1.53	1.46
1	A	105	HIS	ND1-CE1	5.28	1.37	1.32
2	B	379	TRP	N-CA	5.20	1.52	1.46
2	B	364	ALA	C-O	5.12	1.30	1.23
1	A	82	LYS	C-O	5.04	1.30	1.23
2	B	157	PRO	CA-C	5.03	1.56	1.52
2	B	81	ASP	C-O	-5.02	1.18	1.24
1	A	47	GLY	N-CA	5.02	1.52	1.45

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	ARG	NE-CZ-NH1	16.14	137.64	121.50
1	A	140	ARG	NE-CZ-NH2	-15.57	105.19	119.20
1	A	140	ARG	CD-NE-CZ	14.09	144.13	124.40
1	A	90	VAL	N-CA-C	10.80	121.64	110.62
1	A	140	ARG	CB-CG-CD	10.08	134.48	111.30
1	A	130	ARG	NE-CZ-NH2	-7.39	112.55	119.20
1	A	157	ALA	N-CA-C	6.30	120.16	112.23
2	B	263	GLN	N-CA-C	-6.18	104.46	111.14
2	B	81	ASP	CA-C-N	5.87	125.48	119.56
2	B	81	ASP	C-N-CA	5.87	125.48	119.56
2	B	384	GLU	CB-CG-CD	5.64	122.18	112.60
2	B	376	ALA	N-CA-C	5.58	116.72	109.64
2	B	147	GLY	N-CA-C	-5.33	107.17	114.64
2	B	75	ASP	N-CA-C	-5.33	100.04	108.14
1	A	141	ARG	NE-CZ-NH2	-5.13	114.58	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	393	ASN	N-CA-C	5.03	116.76	111.28

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	1370	0	1341	49	0
2	B	3015	0	2959	27	0
3	A	90	0	40	14	0
4	A	12	0	16	0	0
4	B	6	0	8	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
6	B	53	0	30	2	0
7	A	186	0	0	10	0
7	B	367	0	0	5	0
All	All	5107	0	4394	77	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 9.

All (77) 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:B:42:CYS:SG	6:B:501:FAD:C8M	2.03	1.45
1:A:11:CYS:SG	3:A:201:HEC:CAB	2.06	1.44
1:A:14:CYS:SG	3:A:201:HEC:CAC	2.09	1.39
1:A:148:ALA:HB1	1:A:152:LYS:NZ	1.34	1.38
1:A:11:CYS:SG	3:A:201:HEC:CBB	2.30	1.20
2:B:184:LYS:HE2	7:B:967:HOH:O	1.42	1.19
1:A:14:CYS:SG	3:A:201:HEC:CBC	2.48	1.02
1:A:148:ALA:HB1	1:A:152:LYS:HZ2	1.23	1.01
1:A:148:ALA:HB1	1:A:152:LYS:HZ3	1.24	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:CYS:SG	3:A:201:HEC:HBB3	2.07	0.94
3:A:202[A]:HEC:O1D	7:A:455:HOH:O	1.86	0.92
1:A:140:ARG:HD3	7:A:330:HOH:O	1.70	0.91
1:A:14:CYS:SG	3:A:201:HEC:HAC	2.13	0.87
1:A:11:CYS:SG	3:A:201:HEC:HAB	2.16	0.86
1:A:140:ARG:CD	7:A:330:HOH:O	2.22	0.85
2:B:99:ARG:HH11	2:B:290:HIS:HE1	1.23	0.85
1:A:148:ALA:CB	1:A:152:LYS:NZ	2.31	0.83
1:A:97:HIS:HE1	1:A:102:GLU:OE1	1.65	0.79
1:A:14:CYS:SG	3:A:201:HEC:HBC3	2.28	0.73
2:B:99:ARG:HH11	2:B:290:HIS:CE1	2.08	0.71
1:A:14:CYS:SG	3:A:201:HEC:C3C	2.81	0.68
1:A:154:LEU:HD11	1:A:166:LEU:HD11	1.77	0.67
1:A:11:CYS:SG	3:A:201:HEC:C3B	2.85	0.64
2:B:42:CYS:SG	6:B:501:FAD:C8	2.84	0.64
1:A:140:ARG:HD2	7:A:330:HOH:O	1.95	0.62
2:B:151:ILE:HD13	2:B:186:ILE:HB	1.80	0.62
2:B:297:ASN:ND2	7:B:694:HOH:O	2.27	0.60
1:A:148:ALA:CB	1:A:152:LYS:HZ3	2.06	0.59
2:B:66:ARG:NH2	7:B:828:HOH:O	2.12	0.59
1:A:148:ALA:HB1	1:A:152:LYS:HZ1	1.55	0.57
3:A:202[A]:HEC:CGD	7:A:455:HOH:O	2.48	0.57
1:A:154:LEU:C	1:A:154:LEU:HD23	2.30	0.57
1:A:67:GLN:NE2	7:A:425:HOH:O	2.39	0.56
1:A:75:GLN:HG2	7:A:459:HOH:O	2.06	0.55
1:A:71:GLU:HB3	7:A:419:HOH:O	2.08	0.54
1:A:97:HIS:CE1	1:A:102:GLU:OE1	2.55	0.54
2:B:81:ASP:OD2	2:B:84:LYS:HG3	2.07	0.54
1:A:148:ALA:CB	1:A:152:LYS:HZ2	2.05	0.54
2:B:102:VAL:HG12	2:B:104:PRO:HD3	1.90	0.54
1:A:154:LEU:CD1	1:A:166:LEU:HD11	2.38	0.53
2:B:280:THR:O	2:B:290:HIS:HD2	1.92	0.53
2:B:20:TYR:CZ	2:B:313:LYS:HE2	2.43	0.52
2:B:273:TRP:HB2	2:B:297:ASN:ND2	2.25	0.51
1:A:97:HIS:HD2	1:A:170:TYR:OH	1.94	0.51
1:A:9:ASN:HB3	2:B:313:LYS:HD3	1.95	0.48
1:A:85:PHE:CE1	1:A:87:LYS:HD2	2.49	0.47
2:B:60:VAL:HG11	2:B:400:PHE:CG	2.48	0.47
2:B:179:HIS:C	2:B:180:LYS:HG2	2.40	0.47
1:A:2:PRO:HB2	1:A:7:LEU:HG	1.97	0.46
1:A:146:LYS:HA	1:A:146:LYS:HD3	1.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:GLU:O	2:B:74:HIS:HA	2.16	0.45
1:A:11:CYS:CB	3:A:201:HEC:CAB	2.92	0.44
1:A:74[A]:LYS:NZ	7:A:395:HOH:O	2.52	0.43
2:B:66:ARG:NE	7:B:828:HOH:O	2.47	0.43
2:B:37:GLU:HA	2:B:74:HIS:CE1	2.53	0.43
1:A:97:HIS:CD2	1:A:101:CYS:HB2	2.53	0.42
2:B:108:LEU:HB3	2:B:254:PRO:HG2	2.02	0.42
2:B:127:ALA:HA	2:B:133:GLN:HB3	2.03	0.41
2:B:234:ALA:O	2:B:246:LYS:NZ	2.54	0.41
2:B:99:ARG:HD3	2:B:290:HIS:HE1	1.86	0.41
2:B:324:LYS:HG3	7:B:774:HOH:O	2.20	0.41
1:A:149:SER:O	1:A:153:GLU:HG3	2.20	0.41
2:B:371:ILE:O	2:B:372:THR:C	2.63	0.41
1:A:78:TYR:HE2	7:A:429:HOH:O	2.04	0.40
2:B:218:GLU:OE1	2:B:220:HIS:HE1	2.03	0.40
1:A:14:CYS:CB	3:A:201:HEC:C3C	2.99	0.40
2:B:99:ARG:HD3	2:B:290:HIS:CE1	2.57	0.40
1:A:130:ARG:HG2	1:A:167:PHE:CE2	2.56	0.40
1:A:153:GLU:HA	1:A:156:LYS:HE2	2.04	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	173/174 (99%)	171 (99%)	1 (1%)	1 (1%)	21	6
2	B	396/401 (99%)	388 (98%)	8 (2%)	0	100	100
All	All	569/575 (99%)	559 (98%)	9 (2%)	1 (0%)	43	22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	ILE

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	142/141 (101%)	142 (100%)	0	100	100
2	B	310/310 (100%)	307 (99%)	3 (1%)	68	45
All	All	452/451 (100%)	449 (99%)	3 (1%)	76	57

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	43	TYR
2	B	180	LYS
2	B	333	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
1	A	174	GLN
2	B	220	HIS
2	B	290	HIS
2	B	297	ASN
2	B	335	ASN
2	B	386	GLN
2	B	397	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	$\# Z > 2$
2	CSS	B	161	2	4,6,7	0.81	0	2,6,8	1.22	0
2	CSS	B	337	2	4,6,7	0.70	0	2,6,8	2.01	1 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSS	B	161	2	-	0/1/5/7	-
2	CSS	B	337	2	-	0/1/5/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	337	CSS	CA-CB-SG	-2.49	104.23	114.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

9 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	GOL	A	204	-	5,5,5	0.67	0	5,5,5	0.84	0
5	NO3	B	503	-	1,3,3	0.80	0	0,3,3	-	-
3	HEC	A	202[B]	-	46,50,50	2.27	15 (32%)	58,82,82	2.92	27 (46%)
4	GOL	A	203	-	5,5,5	1.51	0	5,5,5	0.93	0
3	HEC	A	202[A]	-	46,50,50	2.25	14 (30%)	58,82,82	2.94	27 (46%)
3	HEC	A	201	1	46,50,50	1.78	12 (26%)	58,82,82	1.79	18 (31%)
4	GOL	B	502	-	5,5,5	1.01	0	5,5,5	0.48	0
6	FAD	B	501	-	58,58,58	1.54	8 (13%)	85,89,89	1.72	19 (22%)
5	NO3	A	205	-	1,3,3	1.54	0	0,3,3	-	-

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	GOL	A	204	-	-	0/4/4/4	-
3	HEC	A	202[B]	-	-	4/14/54/54	-
4	GOL	A	203	-	-	0/4/4/4	-
3	HEC	A	202[A]	-	-	4/14/54/54	-
3	HEC	A	201	1	-	6/14/54/54	-
4	GOL	B	502	-	-	0/4/4/4	-
6	FAD	B	501	-	-	3/34/50/50	0/6/6/6

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	202[A]	HEC	C4C-NC	-5.56	1.29	1.39
3	A	202[B]	HEC	C4C-NC	-5.56	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	202[A]	HEC	C4A-NA	-5.39	1.29	1.39
3	A	202[B]	HEC	C4A-NA	-5.39	1.29	1.39
3	A	202[A]	HEC	CAB-C3B	5.32	1.52	1.35
3	A	202[B]	HEC	CAB-C3B	5.32	1.52	1.35
6	B	501	FAD	P-O3P	4.59	1.64	1.59
3	A	201	HEC	CHA-C1A	4.12	1.46	1.38
3	A	202[A]	HEC	CHA-C4D	4.08	1.48	1.39
3	A	202[B]	HEC	CHA-C4D	4.08	1.48	1.39
3	A	201	HEC	C2A-C3A	3.93	1.45	1.36
6	B	501	FAD	C1'-C2'	-3.90	1.47	1.52
6	B	501	FAD	C8A-N7A	3.80	1.39	1.31
3	A	202[A]	HEC	C4A-C3A	3.69	1.52	1.45
3	A	202[B]	HEC	C4A-C3A	3.69	1.52	1.45
3	A	202[A]	HEC	CAC-C3C	3.43	1.46	1.35
3	A	202[B]	HEC	CAC-C3C	3.43	1.46	1.35
3	A	202[A]	HEC	C1D-ND	-3.39	1.33	1.39
3	A	202[B]	HEC	C1D-ND	-3.39	1.33	1.39
6	B	501	FAD	C7M-C7	3.37	1.57	1.51
3	A	202[A]	HEC	C1B-NB	-3.27	1.33	1.39
3	A	202[B]	HEC	C1B-NB	-3.27	1.33	1.39
3	A	201	HEC	CAB-C3B	3.26	1.45	1.35
3	A	202[A]	HEC	CHD-C1D	3.25	1.46	1.39
3	A	202[B]	HEC	CHD-C1D	3.25	1.46	1.39
6	B	501	FAD	C6-C5X	-3.13	1.35	1.40
3	A	202[A]	HEC	C1A-NA	-3.01	1.33	1.39
3	A	202[B]	HEC	C1A-NA	-3.01	1.33	1.39
3	A	201	HEC	C3B-C4B	-2.87	1.41	1.46
3	A	201	HEC	CHD-C4C	2.84	1.43	1.38
3	A	202[A]	HEC	CHB-C4A	2.79	1.43	1.38
3	A	202[B]	HEC	CHB-C4A	2.79	1.43	1.38
3	A	201	HEC	C4C-NC	-2.79	1.34	1.39
6	B	501	FAD	C1'-N10	2.78	1.54	1.47
3	A	201	HEC	CAC-C3C	2.77	1.44	1.35
3	A	201	HEC	CHB-C4A	2.74	1.43	1.38
3	A	201	HEC	C4A-NA	-2.71	1.34	1.39
3	A	202[A]	HEC	CHB-C1B	2.70	1.45	1.39
3	A	202[B]	HEC	CHB-C1B	2.70	1.45	1.39
3	A	201	HEC	CBA-CGA	2.62	1.56	1.50
6	B	501	FAD	C9A-N10	2.58	1.45	1.41
3	A	202[A]	HEC	CHC-C4B	2.39	1.43	1.38
3	A	202[B]	HEC	CHC-C4B	2.39	1.43	1.38
3	A	202[A]	HEC	C2A-C3A	2.38	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	202[B]	HEC	C2A-C3A	2.38	1.41	1.36
3	A	201	HEC	CHC-C4B	2.36	1.43	1.38
3	A	201	HEC	C1C-C2C	2.15	1.48	1.43
6	B	501	FAD	C5'-C4'	2.10	1.54	1.51
3	A	202[B]	HEC	CBD-CGD	2.06	1.55	1.50

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	202[A]	HEC	C2D-C1D-ND	6.71	120.90	110.14
3	A	202[B]	HEC	C2D-C1D-ND	6.71	120.90	110.14
3	A	202[A]	HEC	C2B-C1B-NB	6.51	120.58	110.14
3	A	202[B]	HEC	C2B-C1B-NB	6.51	120.58	110.14
3	A	202[A]	HEC	CHD-C4C-NC	6.23	131.24	124.45
3	A	202[B]	HEC	CHD-C4C-NC	6.23	131.24	124.45
3	A	202[A]	HEC	CMB-C2B-C1B	6.18	134.83	125.42
3	A	202[B]	HEC	CMB-C2B-C1B	6.18	134.83	125.42
3	A	202[A]	HEC	C3D-C4D-ND	5.85	116.64	110.15
3	A	202[B]	HEC	C3D-C4D-ND	5.85	116.64	110.15
3	A	202[A]	HEC	C1D-C2D-C3D	-5.49	100.53	106.82
3	A	202[B]	HEC	C1D-C2D-C3D	-5.49	100.53	106.82
6	B	501	FAD	C2A-N1A-C6A	5.43	127.65	118.73
6	B	501	FAD	N3A-C2A-N1A	-5.12	120.83	128.58
3	A	202[A]	HEC	CBB-CAB-C3B	-4.80	117.84	127.43
3	A	202[B]	HEC	CBB-CAB-C3B	-4.80	117.84	127.43
6	B	501	FAD	C4A-N9A-C8A	4.72	110.69	105.74
3	A	202[A]	HEC	CMD-C2D-C1D	4.64	132.48	125.42
3	A	202[B]	HEC	CMD-C2D-C1D	4.64	132.48	125.42
3	A	202[A]	HEC	C4D-ND-C1D	-4.63	98.27	105.82
3	A	202[B]	HEC	C4D-ND-C1D	-4.63	98.27	105.82
3	A	201	HEC	CBC-CAC-C3C	-4.44	118.56	127.43
3	A	202[A]	HEC	CMA-C3A-C4A	4.43	132.53	124.73
3	A	202[B]	HEC	CMA-C3A-C4A	4.43	132.53	124.73
3	A	202[A]	HEC	CHB-C4A-C3A	-4.29	116.56	125.49
3	A	202[B]	HEC	CHB-C4A-C3A	-4.29	116.56	125.49
3	A	202[A]	HEC	C4A-C3A-C2A	-4.26	100.65	106.97
3	A	202[B]	HEC	C4A-C3A-C2A	-4.26	100.65	106.97
3	A	202[A]	HEC	CHB-C4A-NA	3.97	128.78	124.45
3	A	202[B]	HEC	CHB-C4A-NA	3.97	128.78	124.45
3	A	202[A]	HEC	C4B-NB-C1B	-3.38	100.32	105.82
3	A	202[B]	HEC	C4B-NB-C1B	-3.38	100.32	105.82
3	A	201	HEC	CHB-C4A-NA	3.36	128.11	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	202[A]	HEC	CHB-C1B-C2B	-3.26	117.97	127.43
3	A	202[B]	HEC	CHB-C1B-C2B	-3.26	117.97	127.43
3	A	202[B]	HEC	CBD-CAD-C3D	-3.22	103.64	112.53
3	A	201	HEC	CHB-C1B-C2B	-3.20	118.14	127.43
6	B	501	FAD	N9A-C8A-N7A	-3.20	109.40	113.94
6	B	501	FAD	C4-C4X-N5	3.19	122.61	118.21
3	A	202[A]	HEC	O2D-CGD-CBD	3.09	123.78	114.00
3	A	201	HEC	O2D-CGD-CBD	3.05	123.64	114.00
3	A	202[A]	HEC	CHD-C4C-C3C	-3.03	120.10	125.21
3	A	202[B]	HEC	CHD-C4C-C3C	-3.03	120.10	125.21
3	A	201	HEC	C1A-C2A-C3A	-3.02	103.13	107.11
3	A	202[A]	HEC	C2A-C1A-NA	2.96	113.18	110.32
3	A	202[B]	HEC	C2A-C1A-NA	2.96	113.18	110.32
6	B	501	FAD	C9A-C5X-N5	-2.93	119.34	122.45
6	B	501	FAD	O4B-C1B-C2B	-2.87	100.47	106.62
6	B	501	FAD	C9A-N10-C10	-2.86	116.40	120.75
6	B	501	FAD	C5X-C9A-N10	2.85	120.54	117.97
3	A	202[A]	HEC	CHD-C1D-C2D	-2.84	119.18	127.43
3	A	202[B]	HEC	CHD-C1D-C2D	-2.84	119.18	127.43
3	A	202[A]	HEC	CAD-CBD-CGD	-2.73	106.43	113.67
3	A	202[A]	HEC	CAD-C3D-C4D	2.71	130.23	124.94
3	A	202[B]	HEC	CAD-C3D-C4D	2.71	130.23	124.94
6	B	501	FAD	C7M-C7-C8	-2.69	115.27	120.76
6	B	501	FAD	C4-N3-C2	-2.69	120.87	125.64
3	A	201	HEC	CHD-C4C-NC	2.68	127.37	124.45
3	A	202[B]	HEC	O2D-CGD-CBD	2.67	122.44	114.00
6	B	501	FAD	C7M-C7-C6	2.65	124.25	119.57
3	A	201	HEC	CBA-CAA-C2A	-2.62	105.30	112.53
3	A	202[A]	HEC	O1D-CGD-CBD	-2.57	114.95	123.09
3	A	201	HEC	CHA-C1A-C2A	-2.53	120.87	124.86
6	B	501	FAD	C6-C5X-C9A	2.51	122.50	119.05
3	A	202[A]	HEC	CMC-C2C-C3C	2.49	132.41	126.55
3	A	202[B]	HEC	CMC-C2C-C3C	2.49	132.41	126.55
3	A	201	HEC	O1D-CGD-CBD	-2.47	115.25	123.09
3	A	201	HEC	CBD-CAD-C3D	-2.45	105.75	112.53
3	A	201	HEC	C2B-C1B-NB	2.43	114.04	110.14
3	A	201	HEC	CHD-C4C-C3C	-2.42	121.13	125.21
3	A	201	HEC	CAA-C2A-C1A	2.41	129.76	124.85
3	A	201	HEC	CHC-C1C-NC	2.41	128.23	123.86
3	A	201	HEC	CHA-C1A-NA	2.36	127.02	124.45
3	A	202[A]	HEC	O2A-CGA-O1A	2.31	129.28	123.33
3	A	202[B]	HEC	O2A-CGA-O1A	2.31	129.28	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	501	FAD	O4B-C1B-N9A	-2.28	103.70	108.09
6	B	501	FAD	C4X-C4-N3	2.27	119.02	113.25
6	B	501	FAD	O5B-C5B-C4B	-2.24	101.38	108.99
3	A	201	HEC	CMB-C2B-C3B	2.19	131.71	126.55
6	B	501	FAD	N6A-C6A-N1A	2.18	123.22	118.38
3	A	202[A]	HEC	CHD-C1D-ND	-2.17	119.92	123.86
3	A	202[B]	HEC	CHD-C1D-ND	-2.17	119.92	123.86
3	A	201	HEC	CBB-CAB-C3B	-2.13	123.18	127.43
3	A	202[A]	HEC	C4D-C3D-C2D	-2.12	103.59	106.87
3	A	202[B]	HEC	C4D-C3D-C2D	-2.12	103.59	106.87
3	A	202[B]	HEC	O1D-CGD-CBD	-2.08	116.49	123.09
6	B	501	FAD	C5A-C4A-N9A	-2.07	103.56	105.81
3	A	201	HEC	CHB-C4A-C3A	-2.04	121.25	125.49
3	A	202[A]	HEC	CHA-C4D-ND	-2.02	120.19	123.86
3	A	202[B]	HEC	CHA-C4D-ND	-2.02	120.19	123.86
6	B	501	FAD	C4'-C3'-C2'	-2.00	110.23	113.57

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	HEC	C2B-C3B-CAB-CBB
3	A	201	HEC	C4B-C3B-CAB-CBB
3	A	201	HEC	C2C-C3C-CAC-CBC
3	A	201	HEC	C4C-C3C-CAC-CBC
3	A	202[A]	HEC	C2C-C3C-CAC-CBC
3	A	202[A]	HEC	C4C-C3C-CAC-CBC
3	A	202[B]	HEC	C2C-C3C-CAC-CBC
3	A	202[B]	HEC	C4C-C3C-CAC-CBC
6	B	501	FAD	O2'-C2'-C3'-O3'
6	B	501	FAD	O2'-C2'-C3'-C4'
3	A	201	HEC	CAD-CBD-CGD-O1D
3	A	202[A]	HEC	CAD-CBD-CGD-O2D
3	A	202[B]	HEC	CAD-CBD-CGD-O1D
3	A	201	HEC	CAD-CBD-CGD-O2D
3	A	202[B]	HEC	CAD-CBD-CGD-O2D
6	B	501	FAD	C1'-C2'-C3'-O3'
3	A	202[A]	HEC	CAD-CBD-CGD-O1D

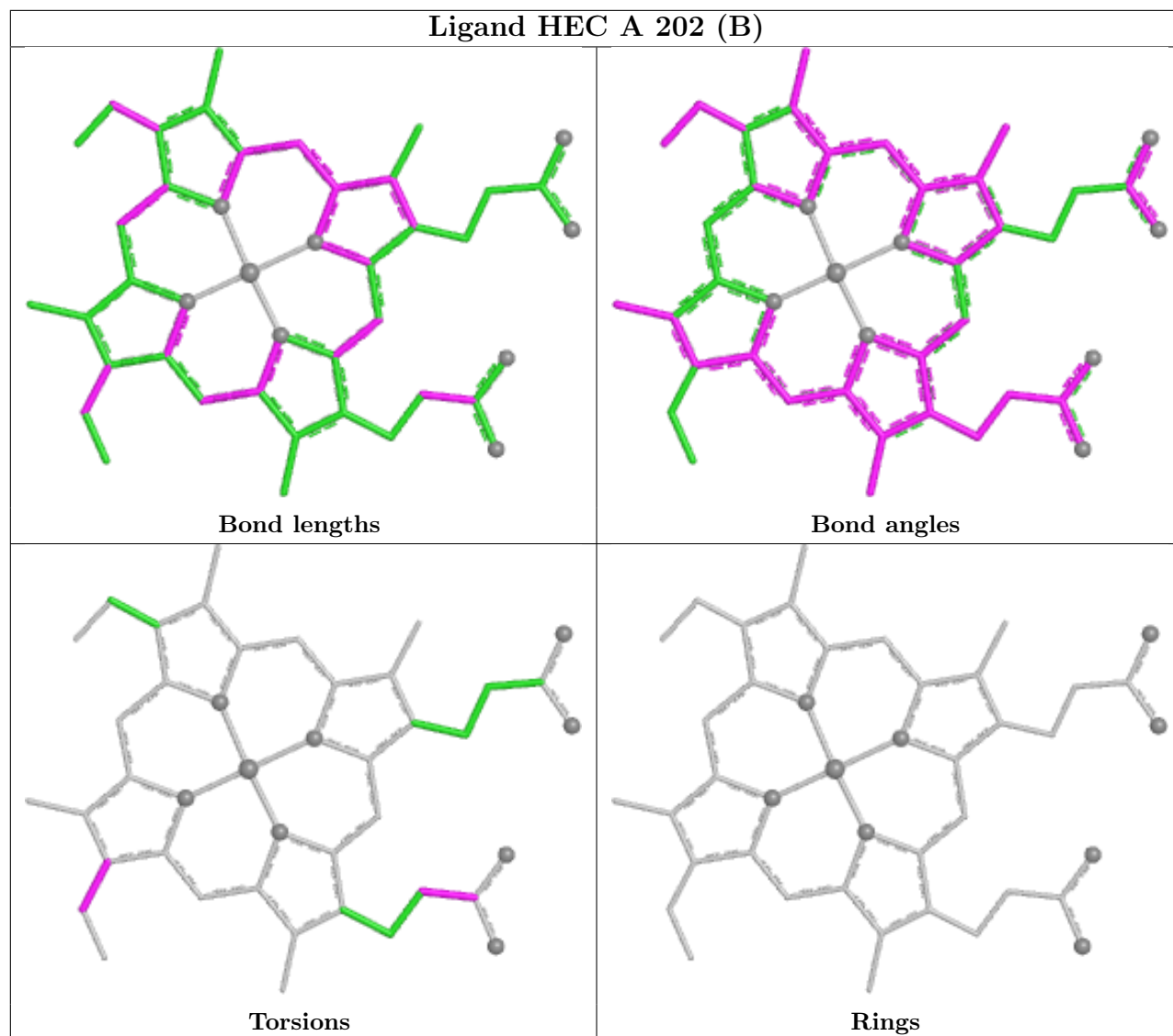
There are no ring outliers.

3 monomers are involved in 16 short contacts:

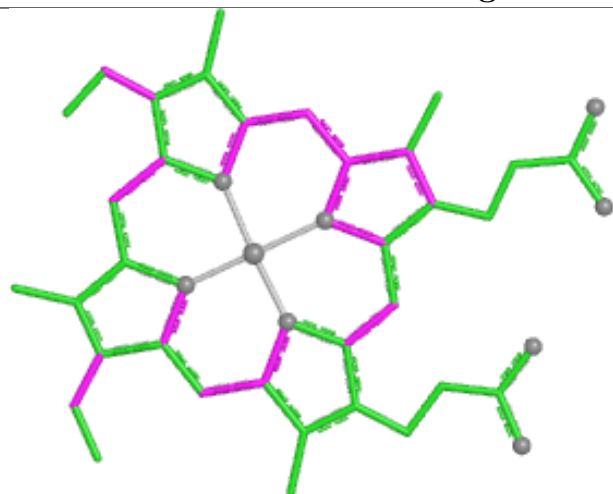
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	202[A]	HEC	2	0
3	A	201	HEC	12	0
6	B	501	FAD	2	0

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.

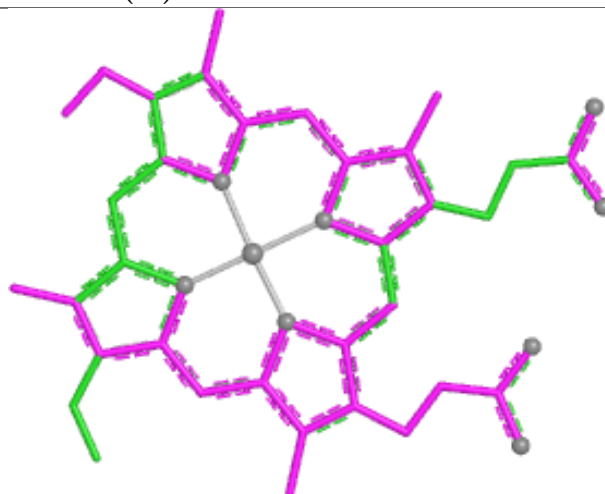
Ligand HEC A 202 (B)



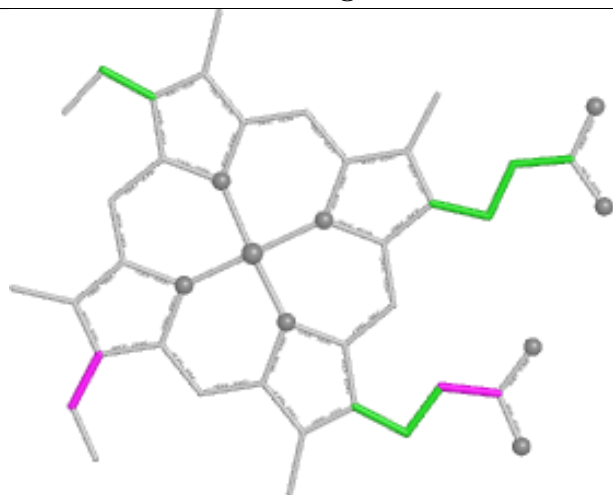
Ligand HEC A 202 (A)



Bond lengths



Bond angles

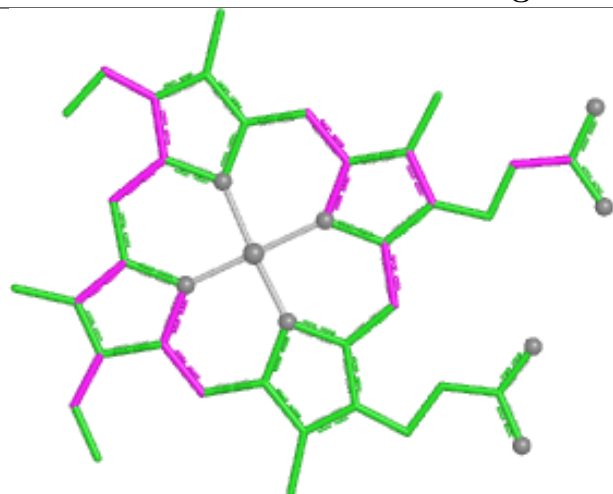


Torsions

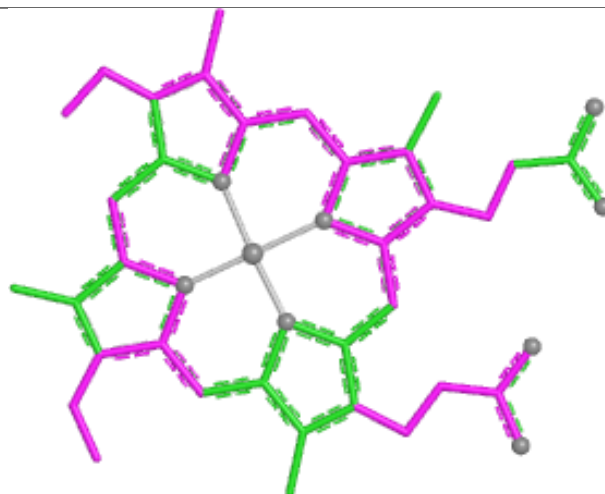


Rings

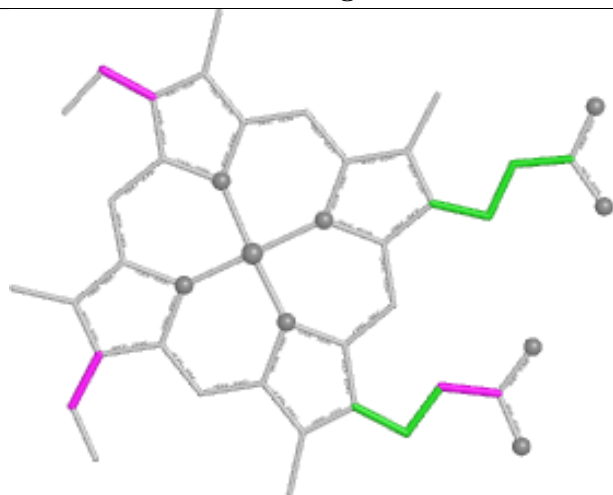
Ligand HEC A 201



Bond lengths



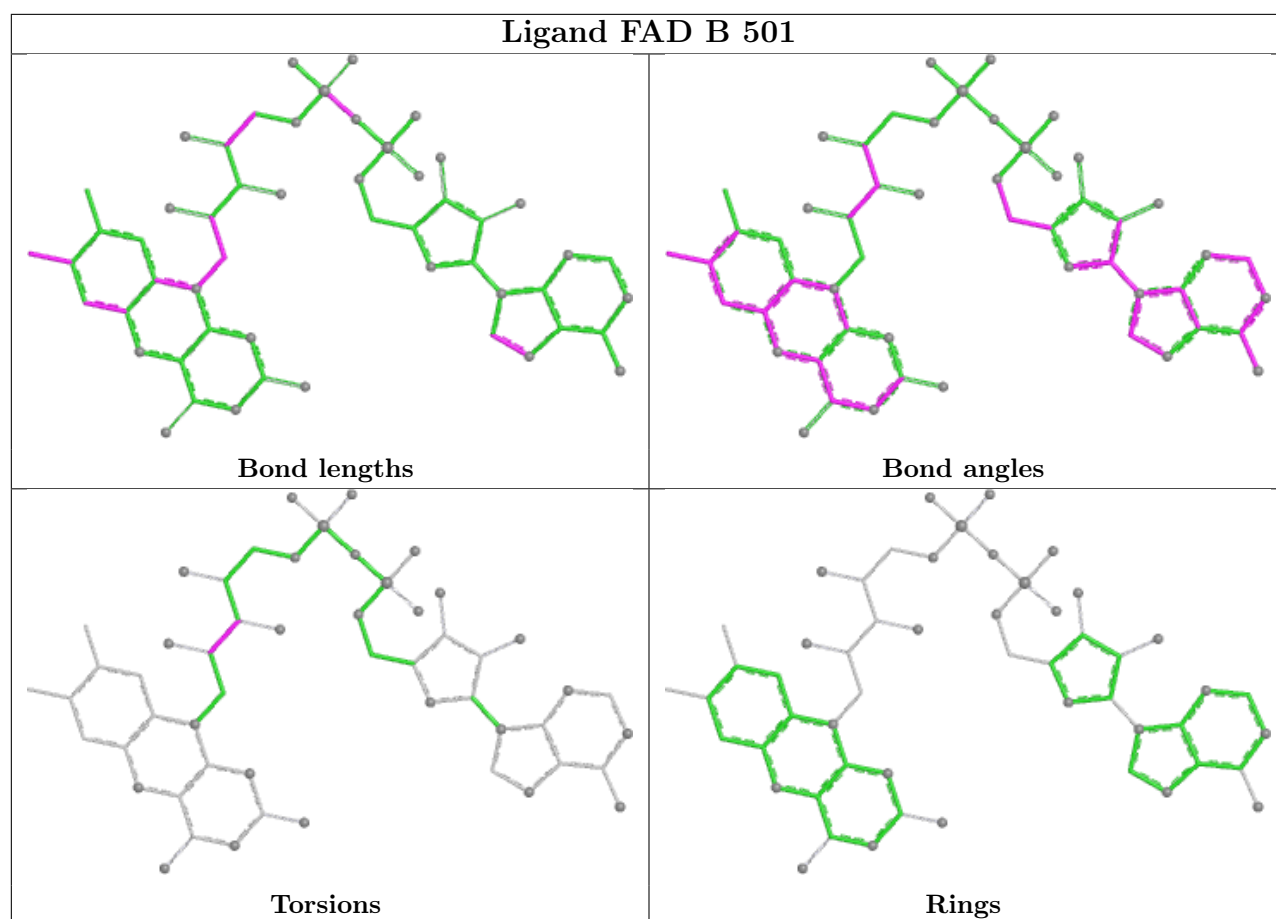
Bond angles



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	174/174 (100%)	-0.21	1 (0%) 85 88	6, 12, 27, 38	1 (0%)
2	B	398/401 (99%)	-0.51	1 (0%) 90 91	5, 10, 20, 34	0
All	All	572/575 (99%)	-0.42	2 (0%) 90 91	5, 10, 24, 38	1 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2	GLY	2.3
1	A	113	ALA	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CSS	B	161	7/8	0.99	0.03	6,6,8,10	0
2	CSS	B	337	7/8	0.99	0.04	5,6,9,11	0

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,

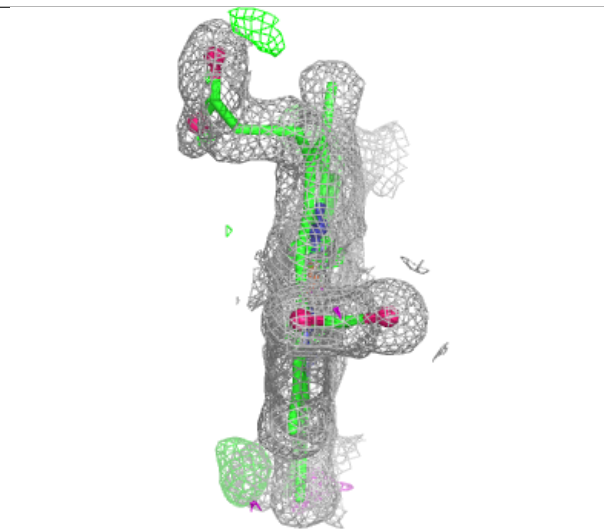
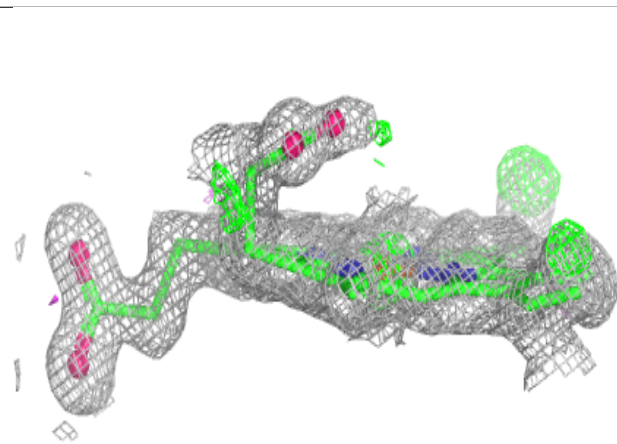
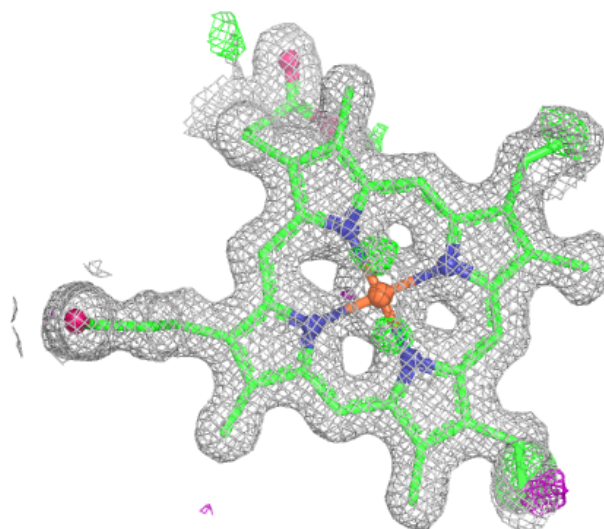
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NO3	B	503	4/4	0.93	0.15	22,25,29,32	0
5	NO3	A	205	4/4	0.94	0.10	18,24,24,30	0
4	GOL	A	203	6/6	0.97	0.04	7,7,9,9	0
4	GOL	B	502	6/6	0.97	0.04	8,10,10,10	0
3	HEC	A	202[B]	43/43	0.98	0.06	8,10,14,23	4
3	HEC	A	202[A]	43/43	0.98	0.06	8,10,16,23	4
4	GOL	A	204	6/6	0.98	0.06	9,11,12,14	0
3	HEC	A	201	43/43	0.99	0.04	5,6,8,11	0
6	FAD	B	501	53/53	0.99	0.03	4,5,8,9	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.

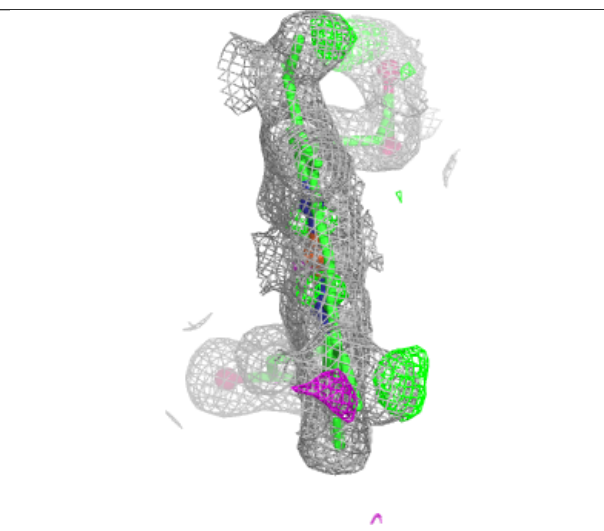
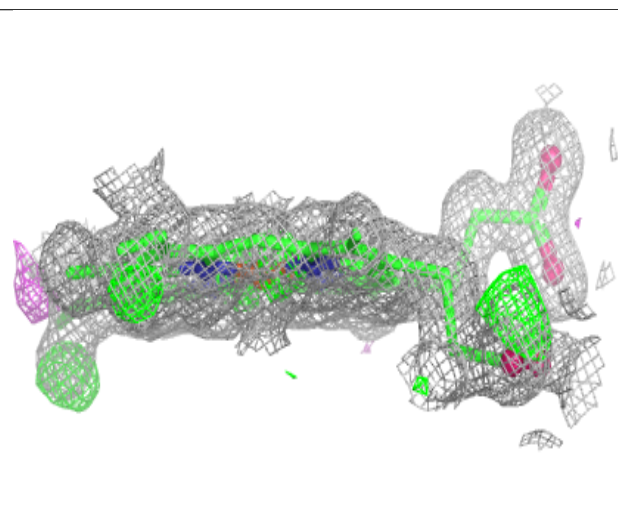
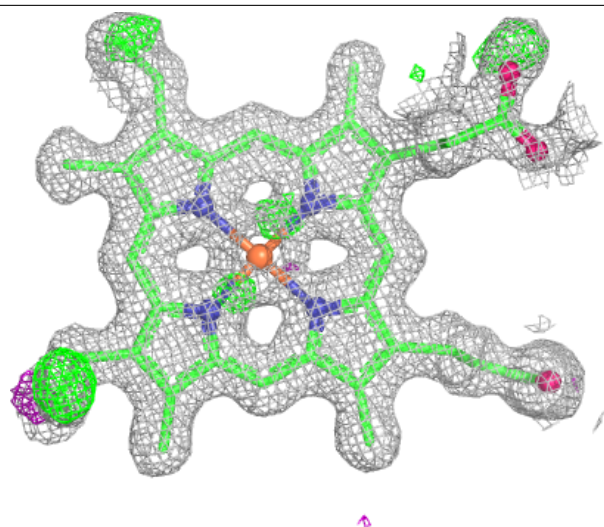
Electron density around HEC A 202 (B):

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



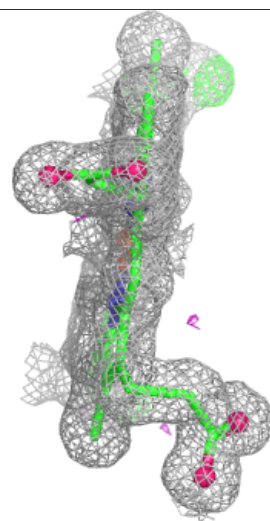
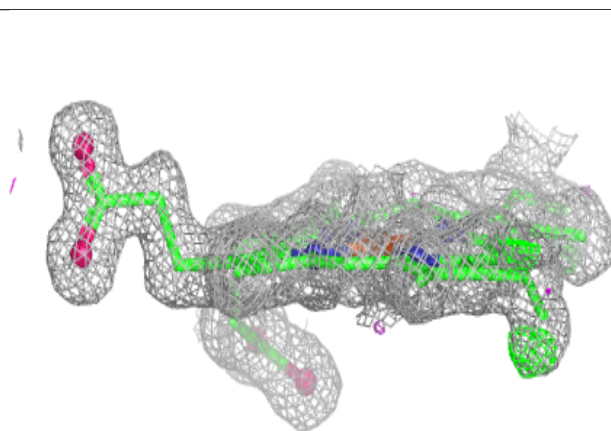
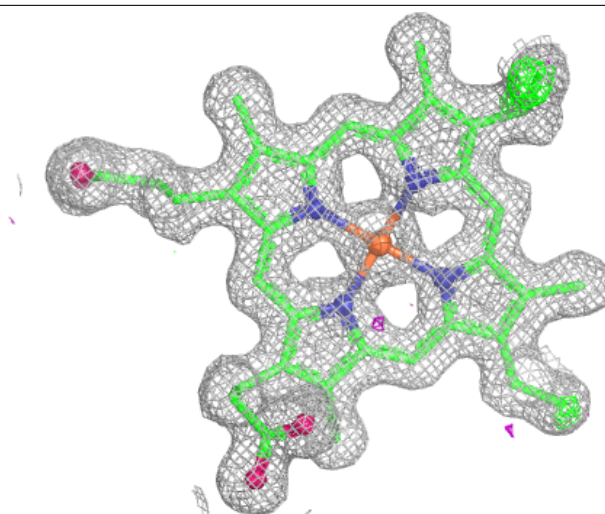
Electron density around HEC A 202 (A):

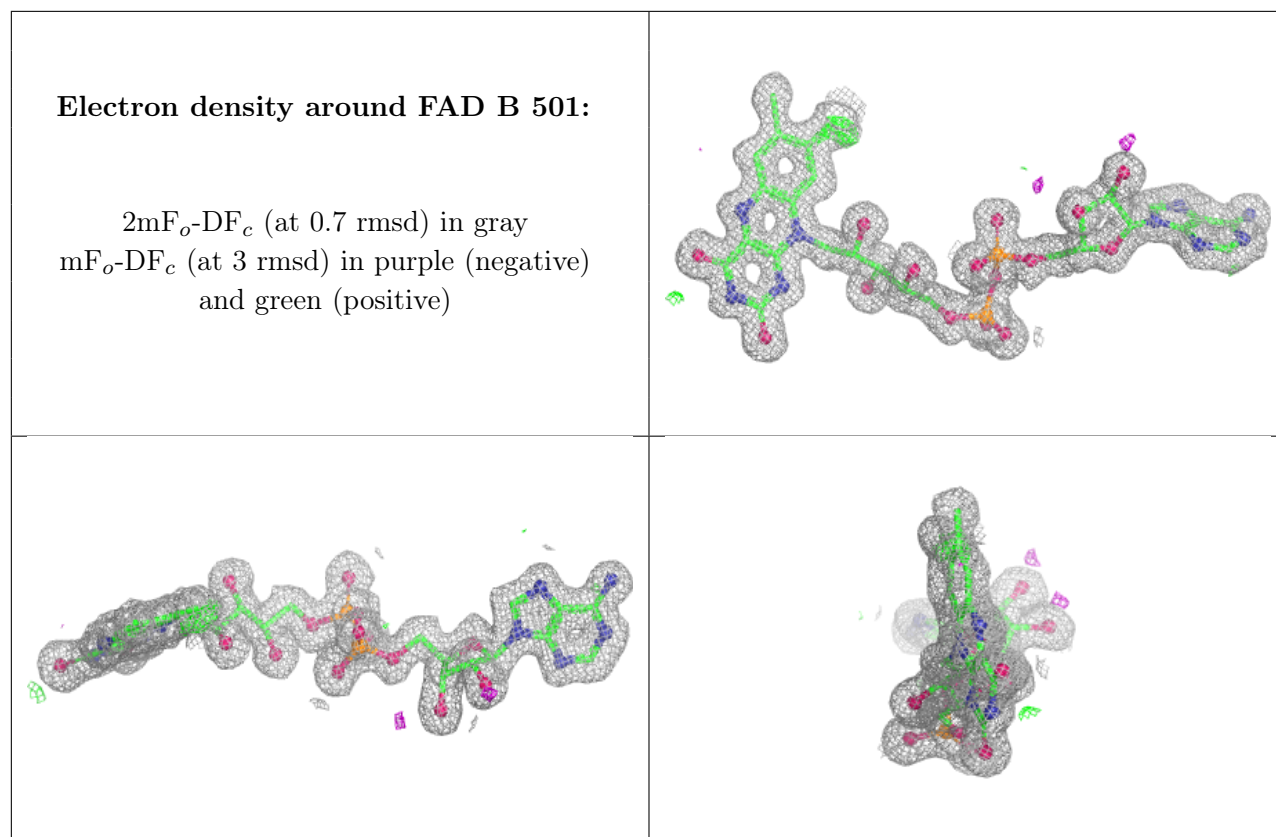
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC A 201:

$2mF_o-DF_c$ (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.