Full wwPDB X-ray Structure Validation Report (i)

Aug 18, 2026 – 08:51 pm BST

PDB ID	:	6FXQ / pdb_00006fxq
Title	:	Structure of coproheme decarboxylase from Listeria monocytogenes during turnover
Authors	:	Hofbauer, S.; Pfanzagl, V.; Mlynek, G.; Puehringer, D.
Deposited on	:	2018-03-09
Resolution	:	1.69 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 (i) 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 (i)) were used in the production of this report:

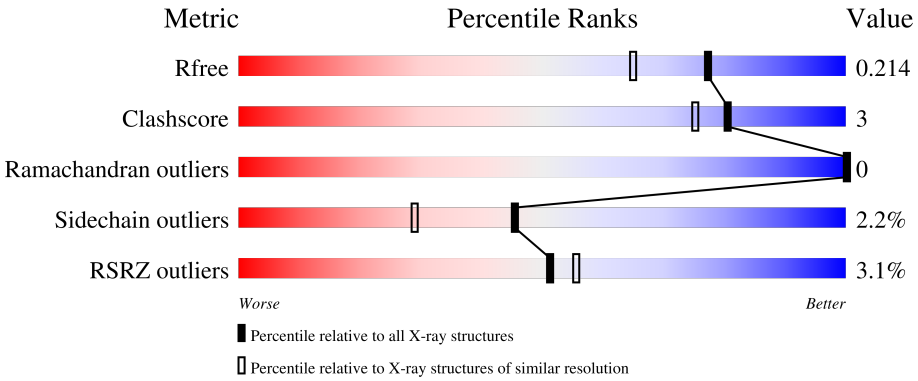
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.69 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	250	4% 96%
1	B	250	2% 88% 5% 7%
1	C	250	4% 88% 6% 5%
1	D	250	3% 96%
1	E	250	2% 91% 6%

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	VOV	A	303[B]	X	-	-	-
4	VOV	B	303[B]	X	-	-	-
4	VOV	C	302[B]	X	-	-	-
4	VOV	D	302[B]	X	-	-	-
4	VOV	E	302[B]	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 20919 atoms, of which 9895 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.

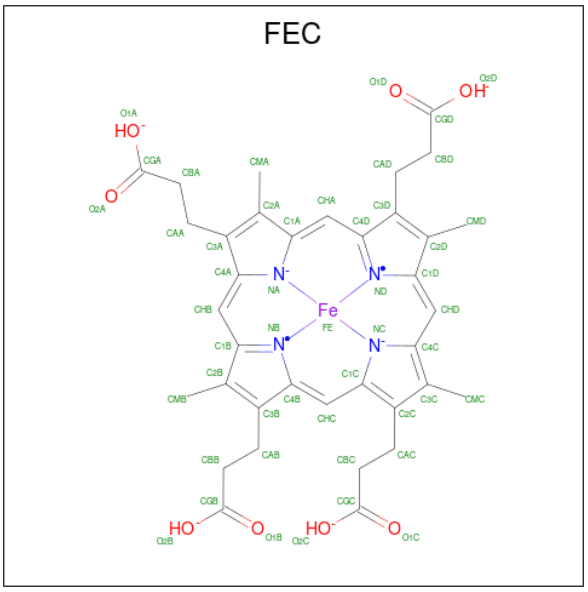
- Molecule 1 is a protein called Putative heme-dependent peroxidase lmo2113.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	248	Total	C	H	N	O	S	0	0	0
			3960	1292	1950	335	374	9			
1	B	233	Total	C	H	N	O	S	0	0	0
			3762	1228	1857	317	352	8			
1	C	237	Total	C	H	N	O	S	0	0	0
			3817	1245	1883	322	359	8			
1	D	250	Total	C	H	N	O	S	0	0	0
			3989	1301	1962	338	379	9			
1	E	235	Total	C	H	N	O	S	0	0	0
			3797	1241	1872	320	356	8			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

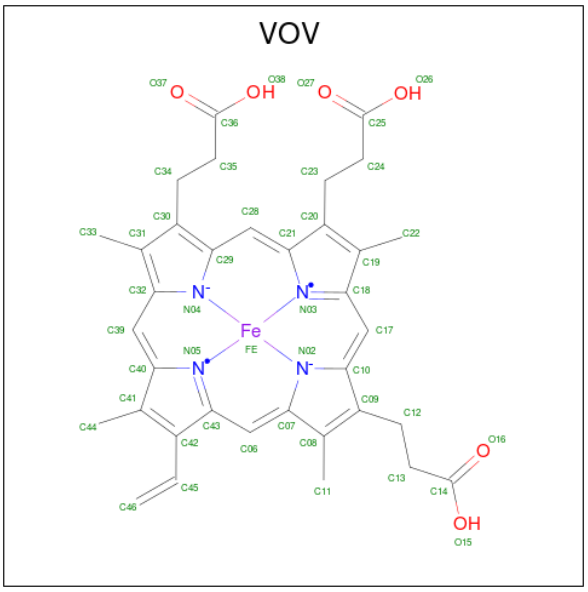
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Na	0	0
			2	2		
2	B	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		
2	D	1	Total	Na	0	0
			1	1		

- Molecule 3 is 1,3,5,8-TETRAMETHYL-PORPHINE-2,4,6,7-TETRAPROPIONIC ACID FERROUS COMPLEX (CCD ID: FEC) (formula: $C_{36}H_{36}FeN_4O_8$) (labeled as "Ligand of Interest" by depositor).



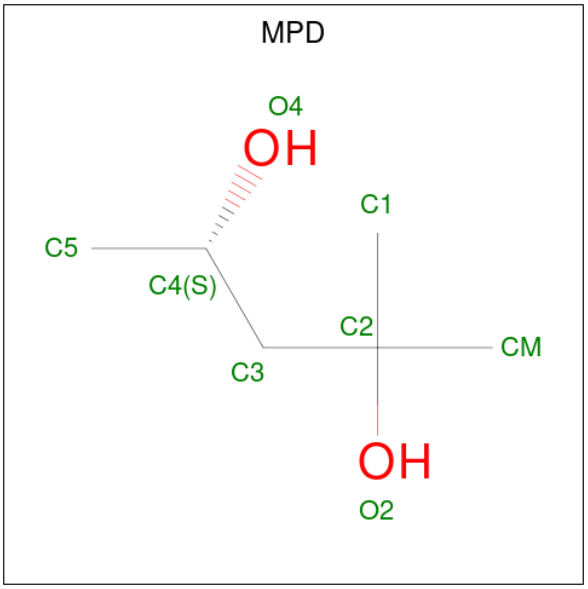
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Fe	H	N	O	0	1
			81	36	1	32	4	8		
3	B	1	Total	C	Fe	H	N	O	0	1
			81	36	1	32	4	8		
3	C	1	Total	C	Fe	H	N	O	0	1
			81	36	1	32	4	8		
3	D	1	Total	C	Fe	H	N	O	0	1
			81	36	1	32	4	8		
3	E	1	Total	C	Fe	H	N	O	0	1
			81	36	1	32	4	8		

- Molecule 4 is harderoheme (III) (CCD ID: VOV) (formula: $C_{35}H_{34}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Fe	H	N	O	0	1
			77	35	1	31	4	6		
4	B	1	Total	C	Fe	H	N	O	0	1
			77	35	1	31	4	6		
4	C	1	Total	C	Fe	H	N	O	0	1
			77	35	1	31	4	6		
4	D	1	Total	C	Fe	H	N	O	0	1
			77	35	1	31	4	6		
4	E	1	Total	C	Fe	H	N	O	0	1
			77	35	1	31	4	6		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			22	6	14	2		
5	B	1	Total	C	H	O	0	0
			22	6	14	2		
5	D	1	Total	C	H	O	0	0
			22	6	14	2		
5	E	1	Total	C	H	O	0	0
			22	6	14	2		

- Molecule 6 is water.

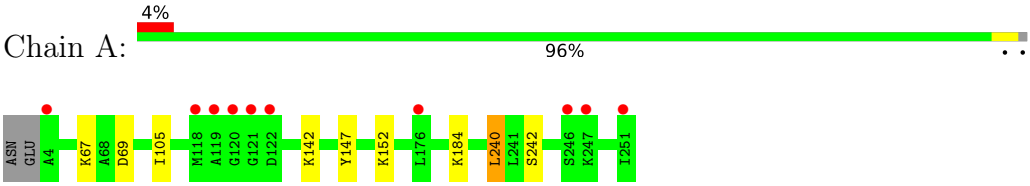
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	148	Total	O	0	0
			148	148		
6	B	123	Total	O	0	0
			123	123		
6	C	128	Total	O	0	0
			128	128		
6	D	165	Total	O	0	0
			165	165		
6	E	147	Total	O	0	0
			147	147		

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.

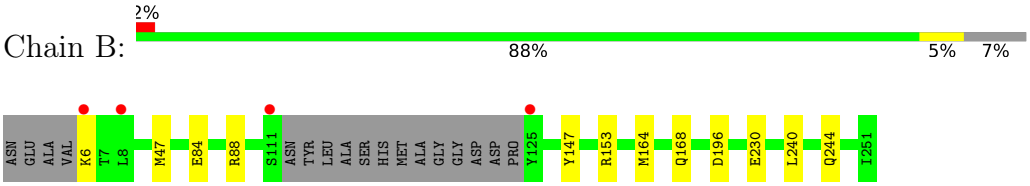
• Molecule 1: Putative heme-dependent peroxidase lmo2113

Chain A:



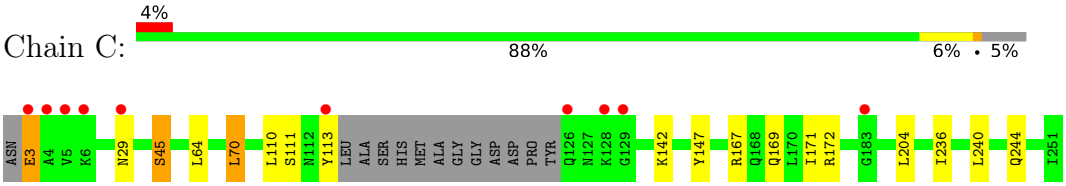
• Molecule 1: Putative heme-dependent peroxidase lmo2113

Chain B:



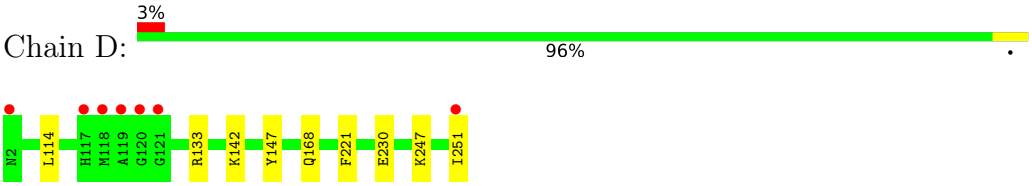
• Molecule 1: Putative heme-dependent peroxidase lmo2113

Chain C:



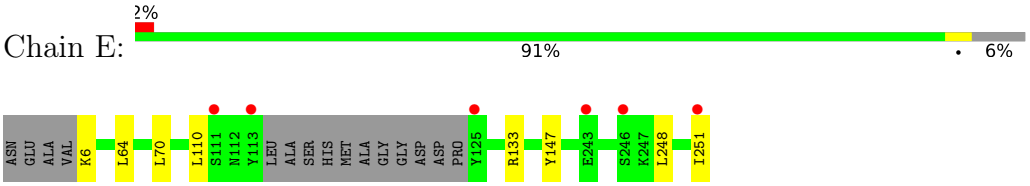
• Molecule 1: Putative heme-dependent peroxidase lmo2113

Chain D:



• Molecule 1: Putative heme-dependent peroxidase lmo2113

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.69Å 129.37Å 77.92Å 90.00° 105.52° 90.00°	Depositor
Resolution (Å)	49.00 – 1.69 49.00 – 1.69	Depositor EDS
% Data completeness (in resolution range)	97.9 (49.00-1.69) 97.9 (49.00-1.69)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.00 (at 1.69Å)	Xtriage
Refinement program	PHENIX dev_2645	Depositor
R, R_{free}	0.178 , 0.214 0.179 , 0.214	Depositor DCC
R_{free} test set	1991 reflections (1.20%)	wwPDB-VP
Wilson B-factor (Å^2)	26.8	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 45.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.033 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	20919	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: FEC, VOV, NA, MPD

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	0/2060	0.68	0/2784
1	B	0.63	0/1951	0.68	0/2633
1	C	0.62	0/1980	0.69	0/2673
1	D	0.65	0/2077	0.71	0/2807
1	E	0.61	0/1972	0.68	0/2662
All	All	0.63	0/10040	0.69	0/13559

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	2010	1950	1950	9	0
1	B	1905	1857	1857	10	0
1	C	1934	1883	1883	15	0
1	D	2027	1962	1962	7	0
1	E	1925	1872	1872	5	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	0	0
3	A	49	32	32	2	0
3	B	49	32	32	5	0
3	C	49	32	32	6	0
3	D	49	32	32	5	0
3	E	49	32	32	7	0
4	A	46	31	0	2	0
4	B	46	31	0	2	0
4	C	46	31	0	0	0
4	D	46	31	0	0	0
4	E	46	31	0	0	0
5	A	8	14	14	0	0
5	B	8	14	14	1	0
5	D	8	14	14	1	0
5	E	8	14	14	1	0
6	A	148	0	0	1	0
6	B	123	0	0	2	0
6	C	128	0	0	1	0
6	D	165	0	0	1	0
6	E	147	0	0	2	0
All	All	11024	9895	9740	52	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 (52) 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:69:ASP:OD1	6:A:401:HOH:O	2.08	0.69
1:C:45:SER:OG	6:C:401:HOH:O	2.14	0.66
5:B:304:MPD:O4	6:B:401:HOH:O	2.15	0.64
3:B:302[A]:FEC:HBB2	3:B:302[A]:FEC:HMB3	1.79	0.64
1:D:147:TYR:OH	3:D:301[A]:FEC:HAD1	2.00	0.60
1:D:168:GLN:OE1	6:D:401:HOH:O	2.17	0.60
1:E:133:ARG:NH2	6:E:403:HOH:O	2.34	0.59
1:A:147:TYR:OH	3:A:302[A]:FEC:HAD1	2.04	0.58
1:A:240:LEU:CD2	6:B:401:HOH:O	2.52	0.56
1:E:147:TYR:OH	3:E:301[A]:FEC:CBD	2.54	0.55
3:E:301[A]:FEC:HBC2	3:E:301[A]:FEC:CHC	2.37	0.55
1:C:113:TYR:CG	1:C:171:ILE:HD13	2.42	0.55
1:D:247:LYS:HD3	5:D:303:MPD:H11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:TYR:OH	3:B:302[A]:FEC:HAD1	2.07	0.54
1:B:147:TYR:OH	3:B:302[A]:FEC:CBD	2.56	0.54
1:C:147:TYR:OH	3:C:301[A]:FEC:CBD	2.56	0.53
1:C:147:TYR:OH	3:C:301[A]:FEC:HBD2	2.08	0.53
1:C:147:TYR:OH	3:C:301[A]:FEC:HAD1	2.08	0.53
1:A:67:LYS:NZ	1:B:196:ASP:OD1	2.43	0.52
1:B:164:MET:HE3	1:B:168:GLN:HG3	1.93	0.51
1:D:147:TYR:OH	3:D:301[A]:FEC:CBD	2.59	0.51
1:E:147:TYR:OH	3:E:301[A]:FEC:HAD1	2.11	0.51
1:C:113:TYR:CD1	1:C:171:ILE:HD13	2.46	0.49
5:E:303:MPD:H13	6:E:452:HOH:O	2.12	0.49
1:A:105:ILE:HG21	1:C:236:ILE:HD11	1.96	0.48
1:E:70:LEU:HD21	1:E:248:LEU:CD2	2.44	0.47
1:B:147:TYR:OH	4:B:303[B]:VOV:C13	2.62	0.47
3:E:301[A]:FEC:HHC	3:E:301[A]:FEC:CBC	2.45	0.46
1:C:169:GLN:HG3	1:C:172:ARG:HH22	1.80	0.46
1:E:147:TYR:OH	3:E:301[A]:FEC:HBD2	2.16	0.46
1:D:147:TYR:OH	3:D:301[A]:FEC:CAD	2.64	0.46
1:C:70:LEU:HD12	1:C:70:LEU:N	2.32	0.44
1:B:147:TYR:OH	4:B:303[B]:VOV:C12	2.67	0.42
3:C:301[A]:FEC:HHA	3:C:301[A]:FEC:HAD2	1.90	0.42
1:D:133:ARG:HH22	3:D:301[A]:FEC:CGB	2.32	0.42
1:A:147:TYR:OH	3:A:302[A]:FEC:CBD	2.68	0.42
1:A:152:LYS:NZ	1:B:153:ARG:O	2.52	0.42
1:B:84:GLU:O	1:B:88:ARG:HG3	2.20	0.42
1:C:3:GLU:HG2	1:D:221:PHE:HB3	2.01	0.41
1:A:147:TYR:OH	4:A:303[B]:VOV:C13	2.67	0.41
1:B:240:LEU:HD23	1:B:244:GLN:CB	2.50	0.41
1:C:240:LEU:HD23	1:C:244:GLN:HB2	2.03	0.41
3:E:301[A]:FEC:CHC	3:E:301[A]:FEC:CBC	2.97	0.41
1:B:147:TYR:OH	3:B:302[A]:FEC:CAD	2.68	0.41
1:C:3:GLU:HG3	1:C:167:ARG:NH2	2.36	0.41
1:C:147:TYR:OH	3:C:301[A]:FEC:CAD	2.69	0.41
1:A:147:TYR:OH	4:A:303[B]:VOV:C12	2.69	0.40
3:D:301[A]:FEC:HHA	3:D:301[A]:FEC:HAD2	1.85	0.40
1:C:240:LEU:HD23	1:C:244:GLN:CB	2.51	0.40
3:E:301[A]:FEC:HHA	3:E:301[A]:FEC:HAD2	1.86	0.40
3:B:302[A]:FEC:HHA	3:B:302[A]:FEC:HAD2	1.83	0.40
1:C:204:LEU:HD21	3:C:301[A]:FEC:HMD3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	246/250 (98%)	243 (99%)	3 (1%)	0	100	100
1	B	229/250 (92%)	227 (99%)	2 (1%)	0	100	100
1	C	233/250 (93%)	228 (98%)	5 (2%)	0	100	100
1	D	248/250 (99%)	246 (99%)	2 (1%)	0	100	100
1	E	231/250 (92%)	226 (98%)	5 (2%)	0	100	100
All	All	1187/1250 (95%)	1170 (99%)	17 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	213/215 (99%)	209 (98%)	4 (2%)	50	34
1	B	203/215 (94%)	200 (98%)	3 (2%)	57	43
1	C	206/215 (96%)	198 (96%)	8 (4%)	28	12
1	D	215/215 (100%)	211 (98%)	4 (2%)	50	34
1	E	205/215 (95%)	201 (98%)	4 (2%)	48	32
All	All	1042/1075 (97%)	1019 (98%)	23 (2%)	45	29

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	LYS
1	A	184	LYS
1	A	240	LEU
1	A	242	SER
1	B	6	LYS
1	B	47	MET
1	B	230	GLU
1	C	3	GLU
1	C	29	ASN
1	C	45	SER
1	C	64	LEU
1	C	70	LEU
1	C	110	LEU
1	C	111	SER
1	C	142	LYS
1	D	114	LEU
1	D	142	LYS
1	D	230	GLU
1	D	251	ILE
1	E	6	LYS
1	E	64	LEU
1	E	110	LEU
1	E	251	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	HIS
1	A	168	GLN
1	B	186	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 5 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
3	FEC	A	302[A]	1	56,56,56	1.42	6 (10%)	76,90,90	1.60	12 (15%)
3	FEC	C	301[A]	-	56,56,56	1.54	8 (14%)	76,90,90	1.38	13 (17%)
4	VOV	D	302[B]	1	53,53,53	1.45	6 (11%)	71,86,86	1.28	8 (11%)
3	FEC	D	301[A]	1	56,56,56	1.54	8 (14%)	76,90,90	1.43	12 (15%)
3	FEC	B	302[A]	-	56,56,56	1.56	8 (14%)	76,90,90	1.49	14 (18%)
4	VOV	B	303[B]	1	53,53,53	1.53	9 (16%)	71,86,86	1.45	14 (19%)
4	VOV	C	302[B]	-	53,53,53	1.44	8 (15%)	71,86,86	1.36	10 (14%)
4	VOV	E	302[B]	1	53,53,53	1.48	12 (22%)	71,86,86	1.38	12 (16%)
4	VOV	A	303[B]	1	53,53,53	1.46	9 (16%)	71,86,86	1.36	9 (12%)
5	MPD	E	303	-	7,7,7	0.48	0	9,10,10	0.62	0
5	MPD	D	303	-	7,7,7	0.40	0	9,10,10	0.50	0
5	MPD	B	304	-	7,7,7	0.54	0	9,10,10	0.47	0
3	FEC	E	301[A]	1	56,56,56	1.57	8 (14%)	76,90,90	1.57	16 (21%)
5	MPD	A	304	-	7,7,7	0.39	0	9,10,10	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FEC	A	302[A]	1	-	4/20/100/100	-
3	FEC	C	301[A]	-	-	4/20/100/100	-
4	VOV	D	302[B]	1	1/1/9/9	6/17/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FEC	D	301[A]	1	-	7/20/100/100	-
4	VOV	C	302[B]	-	1/1/9/9	6/17/57/57	-
4	VOV	B	303[B]	1	1/1/9/9	4/17/57/57	-
4	VOV	E	302[B]	1	1/1/9/9	7/17/57/57	-
3	FEC	B	302[A]	-	-	11/20/100/100	-
4	VOV	A	303[B]	1	1/1/9/9	10/17/57/57	-
5	MPD	E	303	-	-	0/5/5/5	-
5	MPD	D	303	-	-	2/5/5/5	-
5	MPD	B	304	-	-	2/5/5/5	-
3	FEC	E	301[A]	1	-	12/20/100/100	-
5	MPD	A	304	-	-	1/5/5/5	-

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302[A]	FEC	C3B-C2B	6.74	1.51	1.36
3	E	301[A]	FEC	C3B-C2B	6.70	1.51	1.36
3	C	301[A]	FEC	C3B-C2B	6.49	1.50	1.36
3	D	301[A]	FEC	C3B-C2B	6.36	1.50	1.36
3	A	302[A]	FEC	C3B-C2B	5.78	1.49	1.36
4	B	303[B]	VOV	C10-C09	-4.19	1.37	1.45
4	A	303[B]	VOV	C10-C09	-4.05	1.38	1.45
3	D	301[A]	FEC	FE-NB	3.96	2.07	1.94
3	C	301[A]	FEC	FE-NB	3.95	2.07	1.94
3	B	302[A]	FEC	FE-NB	3.86	2.06	1.94
4	D	302[B]	VOV	C10-C09	-3.81	1.38	1.45
4	E	302[B]	VOV	C10-C09	-3.75	1.38	1.45
3	E	301[A]	FEC	FE-NB	3.74	2.06	1.94
4	C	302[B]	VOV	C10-C09	-3.48	1.39	1.45
3	A	302[A]	FEC	FE-NB	3.37	2.05	1.94
3	D	301[A]	FEC	CMA-C2A	3.01	1.57	1.50
3	C	301[A]	FEC	CMC-C3C	2.80	1.56	1.50
4	B	303[B]	VOV	C21-C20	-2.77	1.40	1.45
4	A	303[B]	VOV	C42-C41	2.74	1.42	1.37
4	A	303[B]	VOV	C21-C20	-2.70	1.40	1.45
3	C	301[A]	FEC	CMD-C2D	2.69	1.56	1.50
3	E	301[A]	FEC	CAD-C3D	2.66	1.58	1.51
3	B	302[A]	FEC	CMC-C3C	2.65	1.56	1.50
4	C	302[B]	VOV	C45-C42	2.63	1.54	1.47
4	B	303[B]	VOV	C45-C42	2.62	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301[A]	FEC	CMC-C3C	2.61	1.56	1.50
4	E	302[B]	VOV	C18-C19	-2.60	1.39	1.44
4	B	303[B]	VOV	C09-C08	2.55	1.42	1.36
3	E	301[A]	FEC	CMC-C3C	2.53	1.56	1.50
3	D	301[A]	FEC	CMD-C2D	2.51	1.56	1.50
4	B	303[B]	VOV	C42-C41	2.51	1.42	1.37
4	E	302[B]	VOV	C09-C08	2.49	1.42	1.36
4	D	302[B]	VOV	C21-C20	-2.44	1.40	1.45
4	D	302[B]	VOV	C42-C43	-2.44	1.40	1.44
3	E	301[A]	FEC	CAC-C2C	2.44	1.57	1.51
4	E	302[B]	VOV	C45-C42	2.43	1.54	1.47
3	B	302[A]	FEC	CAD-C3D	2.43	1.57	1.51
4	B	303[B]	VOV	C18-C19	-2.43	1.39	1.44
4	A	303[B]	VOV	C07-C08	-2.43	1.40	1.45
3	B	302[A]	FEC	CMD-C2D	2.40	1.55	1.50
3	C	301[A]	FEC	CMA-C2A	2.40	1.55	1.50
4	C	302[B]	VOV	FE-N03	2.40	2.02	1.94
3	C	301[A]	FEC	CAD-C3D	2.39	1.57	1.51
3	E	301[A]	FEC	CMD-C2D	2.39	1.55	1.50
3	C	301[A]	FEC	FE-NA	2.38	2.03	1.95
3	D	301[A]	FEC	FE-NA	2.37	2.03	1.95
4	E	302[B]	VOV	C21-C20	-2.36	1.41	1.45
4	C	302[B]	VOV	C07-C08	-2.35	1.40	1.45
3	B	302[A]	FEC	CAC-C2C	2.34	1.57	1.51
4	C	302[B]	VOV	C42-C41	2.32	1.42	1.37
3	E	301[A]	FEC	CMA-C2A	2.31	1.55	1.50
3	A	302[A]	FEC	CAC-C2C	2.30	1.57	1.51
3	A	302[A]	FEC	CMD-C2D	2.29	1.55	1.50
4	A	303[B]	VOV	C45-C42	2.25	1.53	1.47
3	A	302[A]	FEC	CMC-C3C	2.24	1.55	1.50
4	E	302[B]	VOV	C29-C30	-2.24	1.40	1.44
4	E	302[B]	VOV	C42-C43	-2.24	1.40	1.44
4	A	303[B]	VOV	FE-N03	2.24	2.01	1.94
3	D	301[A]	FEC	CAD-C3D	2.23	1.57	1.51
4	E	302[B]	VOV	C07-C08	-2.23	1.40	1.45
4	C	302[B]	VOV	C21-C20	-2.22	1.41	1.45
4	B	303[B]	VOV	C40-C41	-2.21	1.40	1.44
3	B	302[A]	FEC	CMA-C2A	2.21	1.55	1.50
3	C	301[A]	FEC	CAC-C2C	2.20	1.57	1.51
3	D	301[A]	FEC	CAC-C2C	2.19	1.57	1.51
4	A	303[B]	VOV	C42-C43	-2.19	1.40	1.44
4	E	302[B]	VOV	C42-C41	2.18	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	302[B]	VOV	C45-C42	2.17	1.53	1.47
4	C	302[B]	VOV	C18-C19	-2.15	1.40	1.44
4	B	303[B]	VOV	C42-C43	-2.14	1.40	1.44
4	D	302[B]	VOV	FE-N03	2.13	2.01	1.94
4	B	303[B]	VOV	FE-N03	2.11	2.01	1.94
3	B	302[A]	FEC	FE-NA	2.11	2.02	1.95
4	C	302[B]	VOV	C29-C30	-2.08	1.40	1.44
4	E	302[B]	VOV	C40-C41	-2.08	1.40	1.44
3	A	302[A]	FEC	CMA-C2A	2.07	1.55	1.50
4	E	302[B]	VOV	FE-N03	2.05	2.01	1.94
3	E	301[A]	FEC	FE-NA	2.02	2.01	1.95
4	A	303[B]	VOV	C09-C08	2.01	1.41	1.36
4	D	302[B]	VOV	C29-C30	-2.01	1.40	1.44
4	A	303[B]	VOV	FE-N05	2.00	2.01	1.94
4	E	302[B]	VOV	FE-N05	2.00	2.01	1.94

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	302[A]	FEC	CBB-CAB-C3B	-4.79	99.32	112.63
3	E	301[A]	FEC	CBD-CAD-C3D	4.26	124.46	112.63
3	B	302[A]	FEC	CBD-CAD-C3D	4.05	123.89	112.63
4	A	303[B]	VOV	O27-C25-C24	-4.04	110.10	123.08
4	D	302[B]	VOV	C23-C24-C25	3.98	122.17	113.60
3	B	302[A]	FEC	CAD-C3D-C2D	3.96	135.25	127.88
3	E	301[A]	FEC	CAD-C3D-C2D	3.91	135.16	127.88
3	B	302[A]	FEC	O2D-CGD-O1D	3.88	132.96	123.30
3	D	301[A]	FEC	O1D-CGD-CBD	-3.83	110.78	123.08
3	A	302[A]	FEC	CBD-CAD-C3D	3.81	123.22	112.63
3	E	301[A]	FEC	O2D-CGD-O1D	3.80	132.76	123.30
3	B	302[A]	FEC	CAD-C3D-C4D	-3.66	118.26	124.66
3	A	302[A]	FEC	C4B-NB-C1B	3.63	108.82	105.07
3	C	301[A]	FEC	CBD-CAD-C3D	3.55	122.49	112.63
3	D	301[A]	FEC	O2D-CGD-O1D	3.49	131.99	123.30
4	C	302[B]	VOV	C23-C20-C21	3.49	130.75	124.66
3	D	301[A]	FEC	O2A-CGA-CBA	-3.48	111.89	123.08
4	C	302[B]	VOV	C23-C24-C25	3.41	120.95	113.60
4	A	303[B]	VOV	C23-C24-C25	3.40	120.92	113.60
3	E	301[A]	FEC	CAD-C3D-C4D	-3.40	118.72	124.66
3	E	301[A]	FEC	O1A-CGA-O2A	3.39	131.76	123.30
4	E	302[B]	VOV	C23-C20-C21	3.35	130.50	124.66
3	C	301[A]	FEC	CBB-CAB-C3B	-3.33	103.37	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	301[A]	FEC	O2D-CGD-O1D	3.32	131.58	123.30
3	A	302[A]	FEC	O1D-CGD-CBD	-3.29	112.50	123.08
3	B	302[A]	FEC	O1A-CGA-O2A	3.29	131.50	123.30
4	B	303[B]	VOV	C23-C20-C21	3.20	130.26	124.66
3	C	301[A]	FEC	CAD-C3D-C2D	3.18	133.80	127.88
4	B	303[B]	VOV	C12-C09-C08	3.18	133.80	127.88
3	C	301[A]	FEC	C4B-NB-C1B	3.14	108.31	105.07
3	D	301[A]	FEC	O1A-CGA-O2A	3.09	130.99	123.30
3	A	302[A]	FEC	O1A-CGA-O2A	3.07	130.96	123.30
3	B	302[A]	FEC	C1B-C2B-C3B	-3.06	103.74	106.96
3	D	301[A]	FEC	CAD-C3D-C2D	3.04	133.54	127.88
3	A	302[A]	FEC	C1B-C2B-C3B	-3.04	103.76	106.96
3	E	301[A]	FEC	O1D-CGD-CBD	-3.03	113.34	123.08
3	A	302[A]	FEC	O2D-CGD-O1D	3.01	130.80	123.30
3	C	301[A]	FEC	CAD-C3D-C4D	-2.99	119.43	124.66
3	B	302[A]	FEC	O1D-CGD-CBD	-2.98	113.50	123.08
4	E	302[B]	VOV	C12-C09-C08	2.97	133.41	127.88
3	A	302[A]	FEC	CAD-C3D-C2D	2.97	133.40	127.88
3	D	301[A]	FEC	C1B-C2B-C3B	-2.96	103.84	106.96
4	B	303[B]	VOV	C23-C24-C25	2.95	119.96	113.60
4	A	303[B]	VOV	C33-C31-C30	2.95	131.98	125.61
4	A	303[B]	VOV	O26-C25-C24	2.94	123.46	114.03
4	E	302[B]	VOV	C23-C24-C25	2.89	119.83	113.60
3	C	301[A]	FEC	O1A-CGA-O2A	2.88	130.47	123.30
3	D	301[A]	FEC	CAD-C3D-C4D	-2.87	119.65	124.66
3	C	301[A]	FEC	C1B-C2B-C3B	-2.86	103.95	106.96
4	E	302[B]	VOV	C12-C13-C14	2.81	119.66	113.60
3	A	302[A]	FEC	CAD-C3D-C4D	-2.81	119.75	124.66
4	B	303[B]	VOV	C12-C13-C14	2.79	119.61	113.60
3	B	302[A]	FEC	C4B-NB-C1B	2.76	107.92	105.07
4	C	302[B]	VOV	C12-C13-C14	2.71	119.43	113.60
4	B	303[B]	VOV	C20-C21-N03	2.68	113.15	110.17
4	C	302[B]	VOV	C41-C40-N05	2.66	112.99	109.84
4	B	303[B]	VOV	C30-C29-N04	2.65	113.11	110.15
3	E	301[A]	FEC	C1B-C2B-C3B	-2.64	104.18	106.96
3	C	301[A]	FEC	O1D-CGD-CBD	-2.63	114.64	123.08
4	D	302[B]	VOV	C23-C20-C21	2.61	129.23	124.66
4	E	302[B]	VOV	C35-C34-C30	-2.61	105.37	112.63
3	E	301[A]	FEC	C4B-NB-C1B	2.61	107.76	105.07
3	E	301[A]	FEC	CAB-C3B-C2B	2.57	132.66	127.88
3	B	302[A]	FEC	O2A-CGA-CBA	-2.54	114.91	123.08
3	B	302[A]	FEC	C1D-ND-C4D	2.52	107.68	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	302[B]	VOV	C41-C40-N05	2.49	112.79	109.84
3	E	301[A]	FEC	O2A-CGA-CBA	-2.47	115.15	123.08
3	A	302[A]	FEC	O2C-CGC-CBC	2.45	121.91	114.03
3	D	301[A]	FEC	CMC-C3C-C2C	2.45	130.91	125.61
4	E	302[B]	VOV	O27-C25-C24	-2.45	115.22	123.08
4	A	303[B]	VOV	C33-C31-C32	-2.44	121.66	125.37
4	E	302[B]	VOV	O37-C36-C35	-2.43	115.28	123.08
4	B	303[B]	VOV	C12-C09-C10	-2.42	120.33	124.89
3	E	301[A]	FEC	C3A-C4A-NA	-2.42	107.97	110.32
4	D	302[B]	VOV	O27-C25-C24	-2.39	115.40	123.08
3	C	301[A]	FEC	CBA-CAA-C3A	2.39	119.26	112.63
3	E	301[A]	FEC	CAB-CBB-CGB	-2.38	108.47	113.60
3	D	301[A]	FEC	CBD-CAD-C3D	2.38	119.25	112.63
3	A	302[A]	FEC	O1B-CGB-CBB	-2.37	115.48	123.08
4	A	303[B]	VOV	C30-C29-N04	2.35	112.77	110.15
3	D	301[A]	FEC	CMC-C3C-C4C	-2.34	121.80	125.37
4	E	302[B]	VOV	C28-C21-N03	-2.33	121.50	124.37
3	D	301[A]	FEC	C2B-C1B-NB	2.33	112.67	109.88
4	C	302[B]	VOV	O27-C25-C24	-2.32	115.61	123.08
4	A	303[B]	VOV	C09-C10-N02	2.31	112.57	110.32
4	D	302[B]	VOV	C41-C40-N05	2.30	112.57	109.84
4	B	303[B]	VOV	C41-C40-N05	2.29	112.55	109.84
3	B	302[A]	FEC	CMD-C2D-C1D	-2.28	121.56	125.04
3	C	301[A]	FEC	O2C-CGC-CBC	2.28	121.35	114.03
3	D	301[A]	FEC	C4B-NB-C1B	2.26	107.41	105.07
4	C	302[B]	VOV	C23-C20-C19	-2.25	123.68	127.88
4	B	303[B]	VOV	O37-C36-C35	-2.23	115.92	123.08
3	A	302[A]	FEC	CAB-CBB-CGB	-2.21	108.84	113.60
4	E	302[B]	VOV	C09-C10-N02	2.20	112.46	110.32
4	A	303[B]	VOV	C20-C21-N03	2.20	112.61	110.17
3	E	301[A]	FEC	CAC-CBC-CGC	2.20	118.33	113.60
4	A	303[B]	VOV	O37-C36-C35	-2.20	116.03	123.08
4	B	303[B]	VOV	C17-C18-N03	-2.19	122.04	124.42
4	E	302[B]	VOV	C23-C20-C19	-2.17	123.84	127.88
3	B	302[A]	FEC	C2B-C1B-NB	2.16	112.47	109.88
3	C	301[A]	FEC	O2A-CGA-CBA	-2.15	116.18	123.08
4	D	302[B]	VOV	C09-C10-N02	2.13	112.40	110.32
4	E	302[B]	VOV	C33-C31-C30	2.12	130.19	125.61
3	E	301[A]	FEC	CMD-C2D-C1D	-2.11	121.83	125.04
4	C	302[B]	VOV	C30-C29-N04	2.11	112.50	110.15
4	C	302[B]	VOV	C33-C31-C30	2.10	130.16	125.61
4	D	302[B]	VOV	C20-C21-N03	2.09	112.50	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	302[B]	VOV	O37-C36-C35	-2.09	116.37	123.08
3	B	302[A]	FEC	CMB-C2B-C3B	2.07	131.72	126.12
4	C	302[B]	VOV	C19-C18-N03	2.06	112.34	109.88
4	B	303[B]	VOV	O27-C25-C24	-2.05	116.50	123.08
3	C	301[A]	FEC	C1D-ND-C4D	2.05	107.19	105.07
4	B	303[B]	VOV	C28-C21-N03	-2.05	121.85	124.37
4	B	303[B]	VOV	C10-N02-C07	2.04	107.35	105.35
3	B	302[A]	FEC	O2C-CGC-CBC	2.03	120.57	114.03
4	B	303[B]	VOV	C19-C18-N03	2.03	112.31	109.88
3	E	301[A]	FEC	CMB-C2B-C3B	2.02	131.61	126.12
3	E	301[A]	FEC	C1D-ND-C4D	2.01	107.15	105.07
4	D	302[B]	VOV	O26-C25-C24	2.01	120.48	114.03
4	D	302[B]	VOV	C34-C35-C36	2.00	117.91	113.60

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	303[B]	VOV	N02
4	B	303[B]	VOV	N02
4	C	302[B]	VOV	N02
4	D	302[B]	VOV	N02
4	E	302[B]	VOV	N02

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302[A]	FEC	C1C-C2C-CAC-CBC
3	B	302[A]	FEC	C4B-C3B-CAB-CBB
3	E	301[A]	FEC	C1C-C2C-CAC-CBC
3	E	301[A]	FEC	C2C-CAC-CBC-CGC
4	A	303[B]	VOV	C29-C30-C34-C35
4	A	303[B]	VOV	C31-C30-C34-C35
4	A	303[B]	VOV	C41-C42-C45-C46
4	A	303[B]	VOV	C43-C42-C45-C46
4	C	302[B]	VOV	C29-C30-C34-C35
4	C	302[B]	VOV	C31-C30-C34-C35
4	D	302[B]	VOV	C41-C42-C45-C46
4	D	302[B]	VOV	C43-C42-C45-C46
5	D	303	MPD	C2-C3-C4-O4
3	B	302[A]	FEC	C2B-C3B-CAB-CBB
3	E	301[A]	FEC	C2B-C3B-CAB-CBB
3	E	301[A]	FEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	B	302[A]	FEC	C3C-C2C-CAC-CBC
3	E	301[A]	FEC	C3C-C2C-CAC-CBC
3	B	302[A]	FEC	C2C-CAC-CBC-CGC
3	E	301[A]	FEC	C2A-C3A-CAA-CBA
4	C	302[B]	VOV	C30-C34-C35-C36
4	E	302[B]	VOV	C09-C12-C13-C14
4	E	302[B]	VOV	C30-C34-C35-C36
3	E	301[A]	FEC	C4A-C3A-CAA-CBA
3	C	301[A]	FEC	C2C-CAC-CBC-CGC
4	B	303[B]	VOV	C09-C12-C13-C14
4	C	302[B]	VOV	C09-C12-C13-C14
4	D	302[B]	VOV	C09-C12-C13-C14
3	C	301[A]	FEC	C3D-CAD-CBD-CGD
5	A	304	MPD	C2-C3-C4-C5
5	D	303	MPD	C2-C3-C4-C5
3	B	302[A]	FEC	C2A-C3A-CAA-CBA
4	A	303[B]	VOV	C09-C12-C13-C14
4	B	303[B]	VOV	C34-C35-C36-O38
4	E	302[B]	VOV	C19-C20-C23-C24
4	B	303[B]	VOV	C34-C35-C36-O37
3	A	302[A]	FEC	CAC-CBC-CGC-O2C
3	D	301[A]	FEC	CAB-CBB-CGB-O2B
3	D	301[A]	FEC	C2D-C3D-CAD-CBD
3	D	301[A]	FEC	CAB-CBB-CGB-O1B
4	A	303[B]	VOV	C34-C35-C36-O37
3	A	302[A]	FEC	CAC-CBC-CGC-O1C
4	A	303[B]	VOV	C34-C35-C36-O38
4	D	302[B]	VOV	C34-C35-C36-O37
3	A	302[A]	FEC	C2D-C3D-CAD-CBD
4	D	302[B]	VOV	C34-C35-C36-O38
4	E	302[B]	VOV	C12-C13-C14-O15
3	B	302[A]	FEC	CAC-CBC-CGC-O2C
3	B	302[A]	FEC	CAC-CBC-CGC-O1C
3	E	301[A]	FEC	CAB-CBB-CGB-O2B
3	B	302[A]	FEC	C4A-C3A-CAA-CBA
4	C	302[B]	VOV	C12-C13-C14-O15
4	E	302[B]	VOV	C34-C35-C36-O38
4	A	303[B]	VOV	C23-C24-C25-O27
3	D	301[A]	FEC	CAA-CBA-CGA-O2A
3	D	301[A]	FEC	CAC-CBC-CGC-O2C
3	E	301[A]	FEC	CAB-CBB-CGB-O1B
4	E	302[B]	VOV	C34-C35-C36-O37

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Mol	Chain	Res	Type	Atoms
3	D	301[A]	FEC	CAC-CBC-CGC-O1C
4	A	303[B]	VOV	C23-C24-C25-O26
3	C	301[A]	FEC	C2A-C3A-CAA-CBA
3	D	301[A]	FEC	CAA-CBA-CGA-O1A
4	A	303[B]	VOV	C12-C13-C14-O15
5	B	304	MPD	C2-C3-C4-C5
4	E	302[B]	VOV	C12-C13-C14-O16
4	C	302[B]	VOV	C12-C13-C14-O16
3	E	301[A]	FEC	CAC-CBC-CGC-O2C
3	E	301[A]	FEC	CAC-CBC-CGC-O1C
3	C	301[A]	FEC	C2D-C3D-CAD-CBD
4	B	303[B]	VOV	C23-C24-C25-O26
5	B	304	MPD	C2-C3-C4-O4
3	A	302[A]	FEC	C4D-C3D-CAD-CBD
4	D	302[B]	VOV	C23-C24-C25-O27
3	E	301[A]	FEC	C2D-C3D-CAD-CBD
3	B	302[A]	FEC	CAB-CBB-CGB-O1B
3	B	302[A]	FEC	CAB-CBB-CGB-O2B

There are no ring outliers.

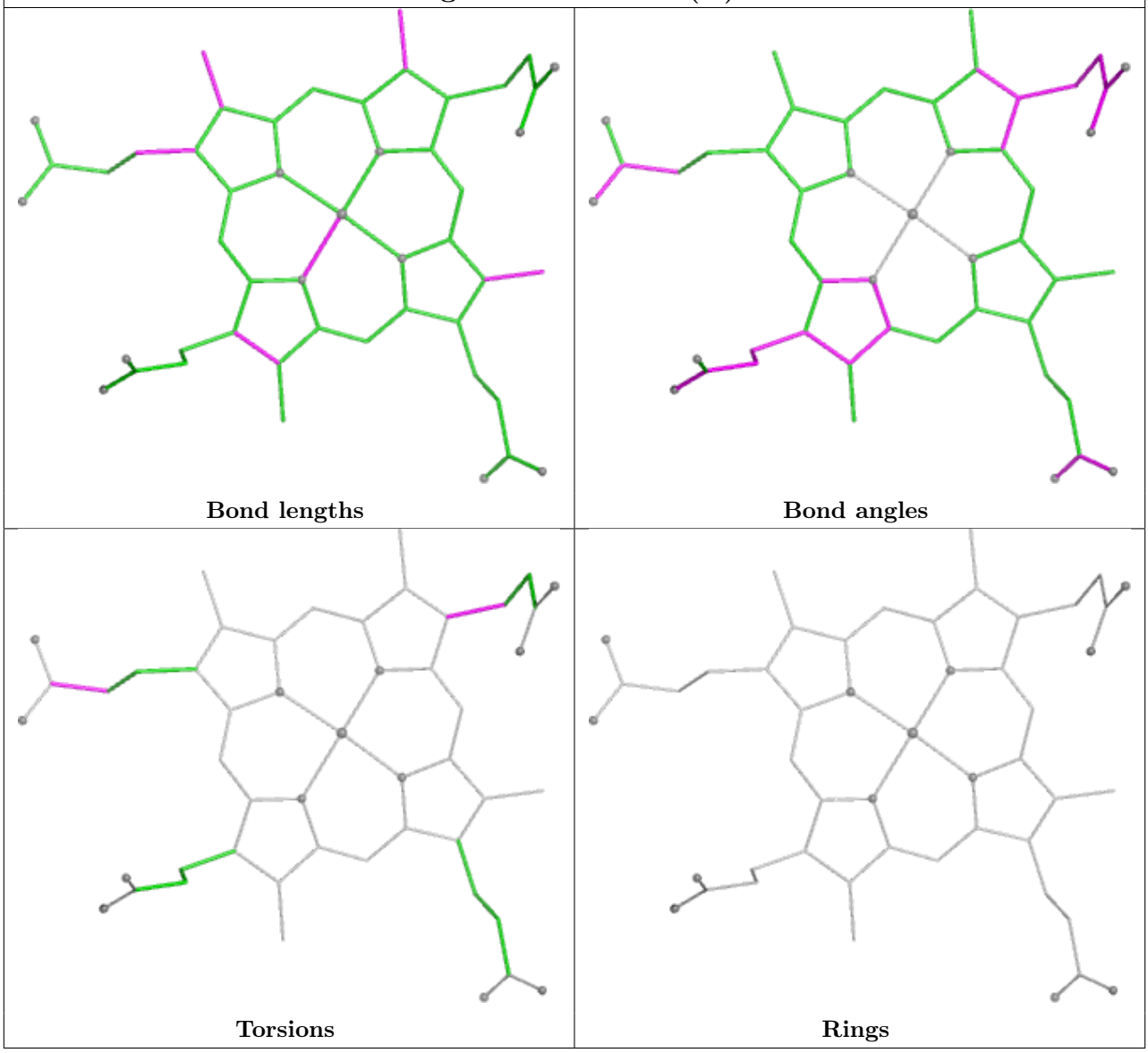
10 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302[A]	FEC	2	0
3	C	301[A]	FEC	6	0
3	D	301[A]	FEC	5	0
3	B	302[A]	FEC	5	0
4	B	303[B]	VOV	2	0
4	A	303[B]	VOV	2	0
5	E	303	MPD	1	0
5	D	303	MPD	1	0
5	B	304	MPD	1	0
3	E	301[A]	FEC	7	0

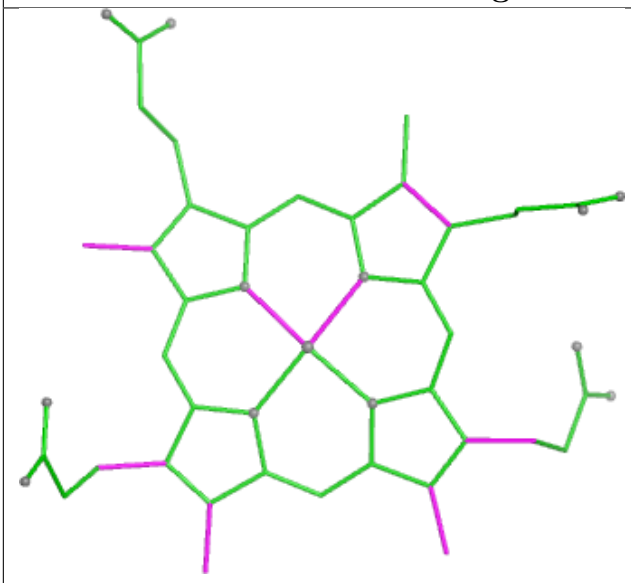
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

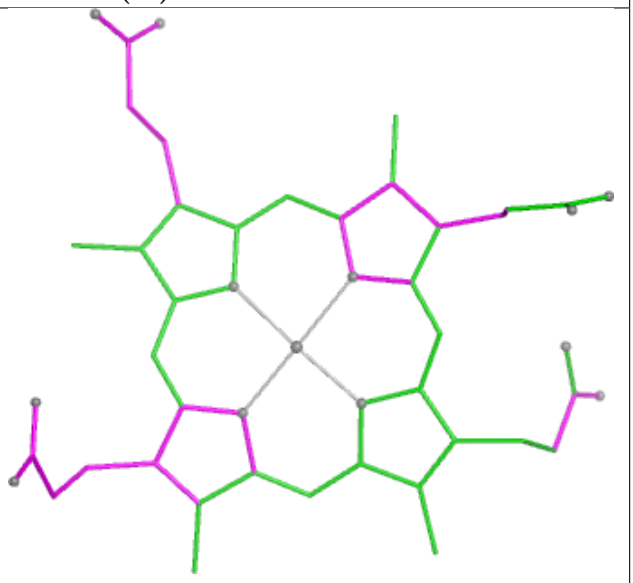
Ligand FEC A 302 (A)



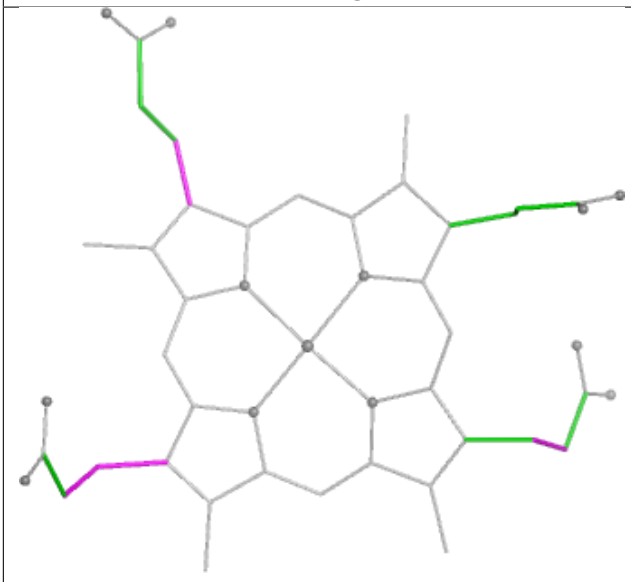
Ligand FEC C 301 (A)



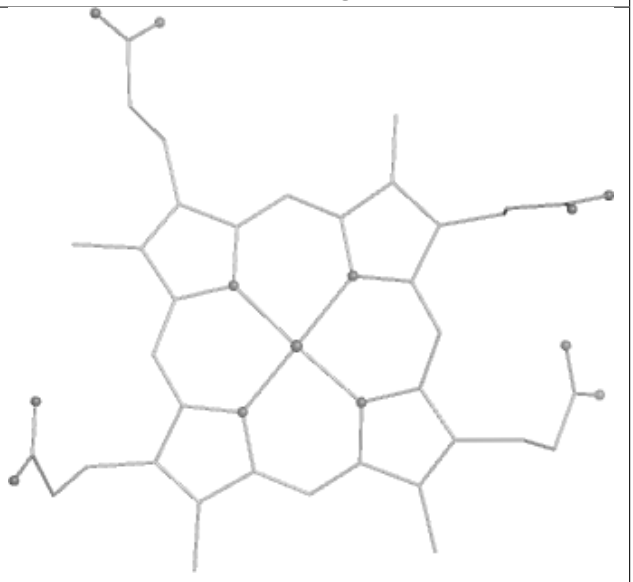
Bond lengths



Bond angles

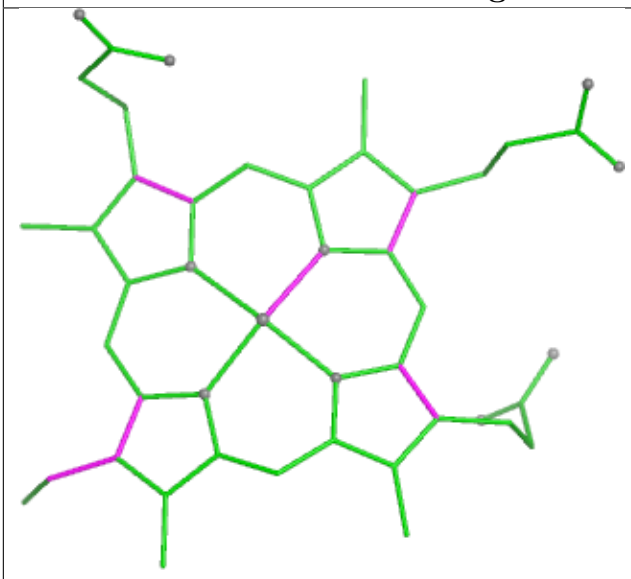


Torsions

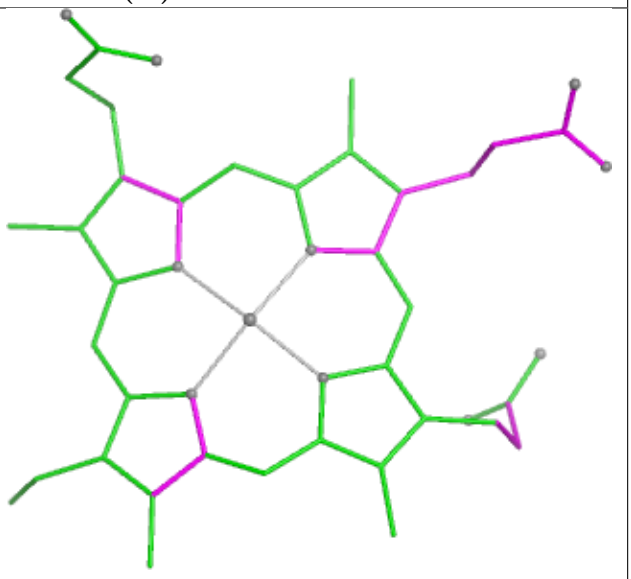


Rings

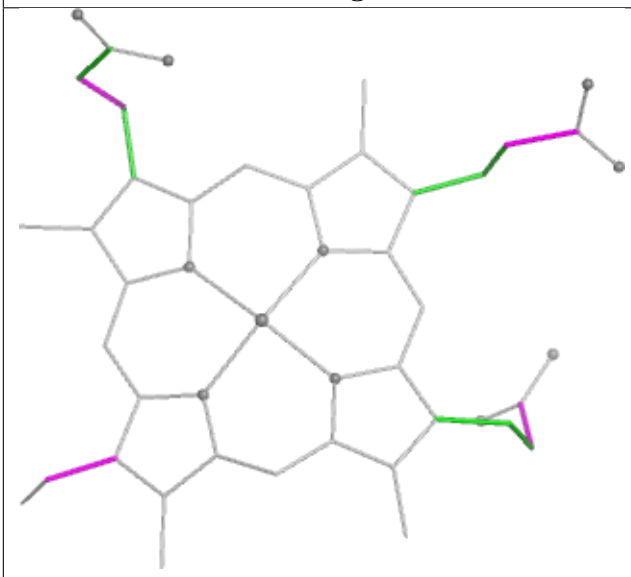
Ligand VOV D 302 (B)



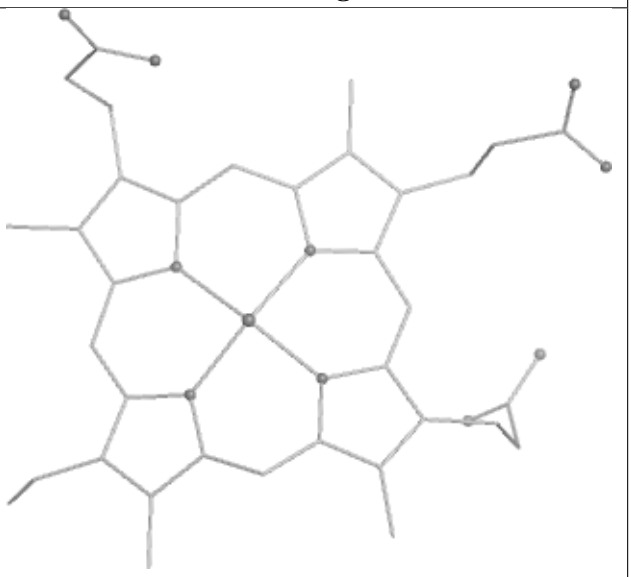
Bond lengths



Bond angles

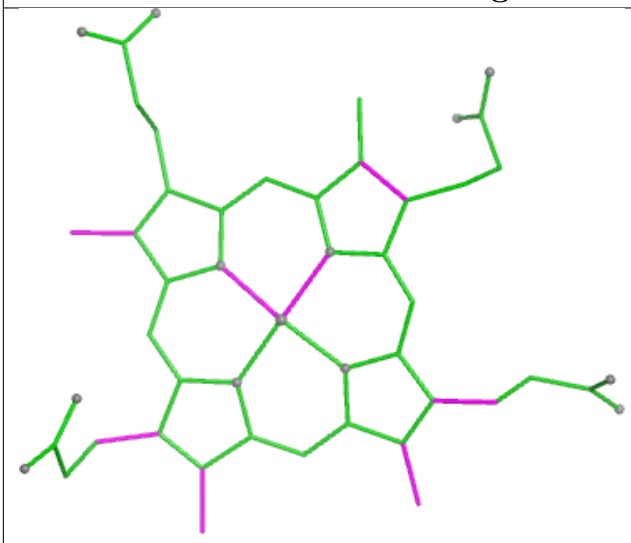


Torsions



Rings

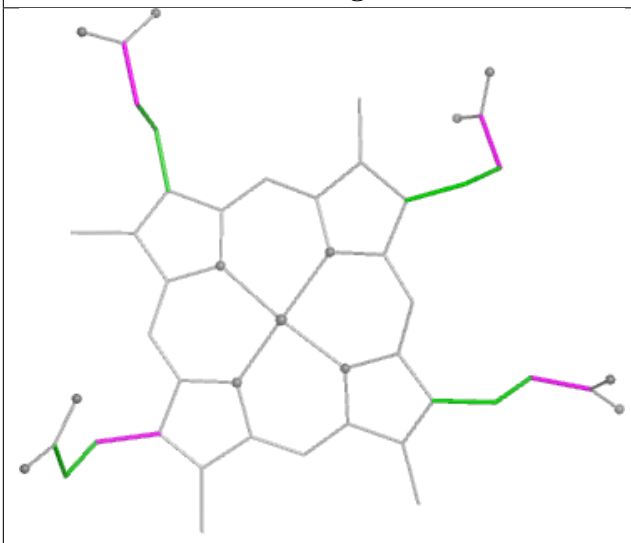
Ligand FEC D 301 (A)



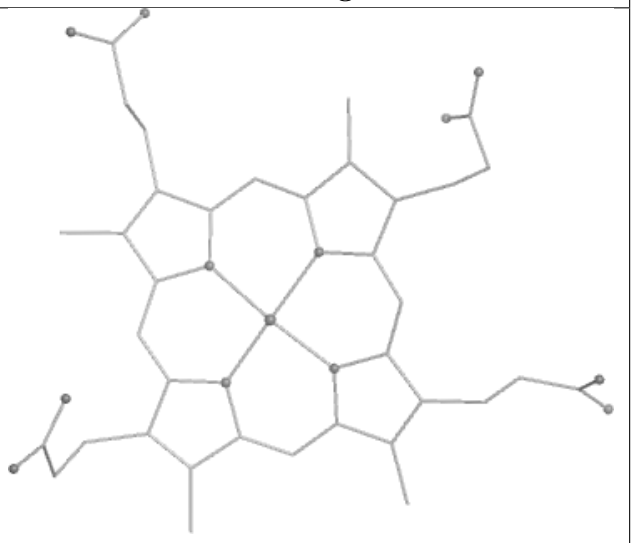
Bond lengths



Bond angles

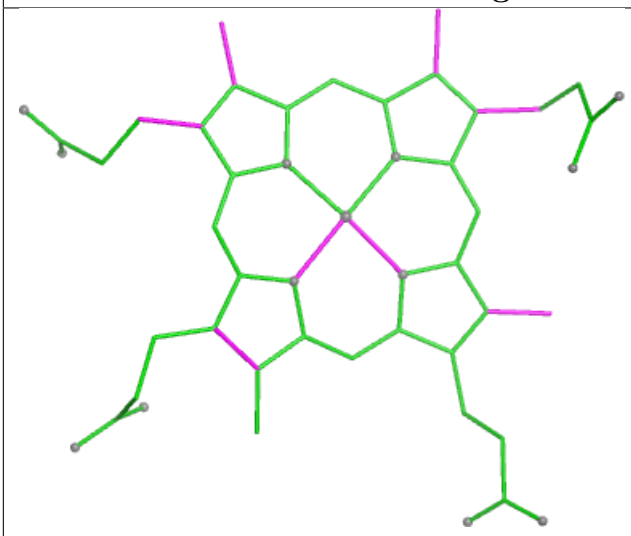


Torsions

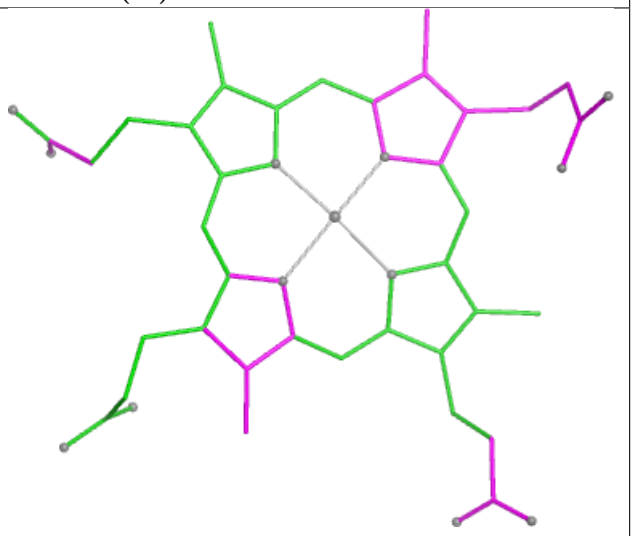


Rings

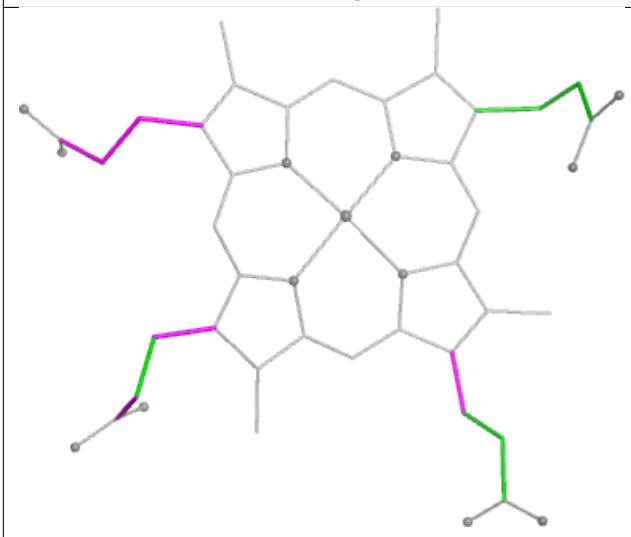
Ligand FEC B 302 (A)



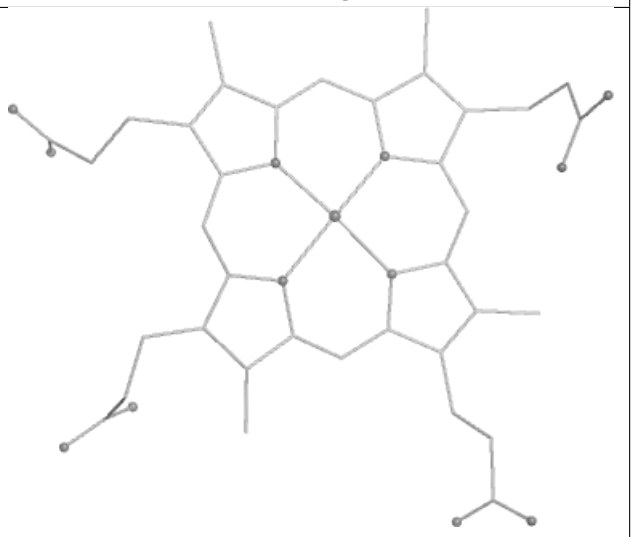
Bond lengths



Bond angles

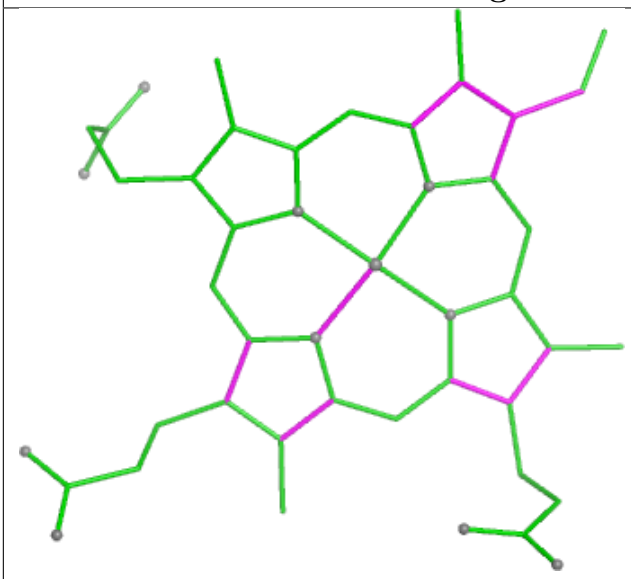


Torsions



Rings

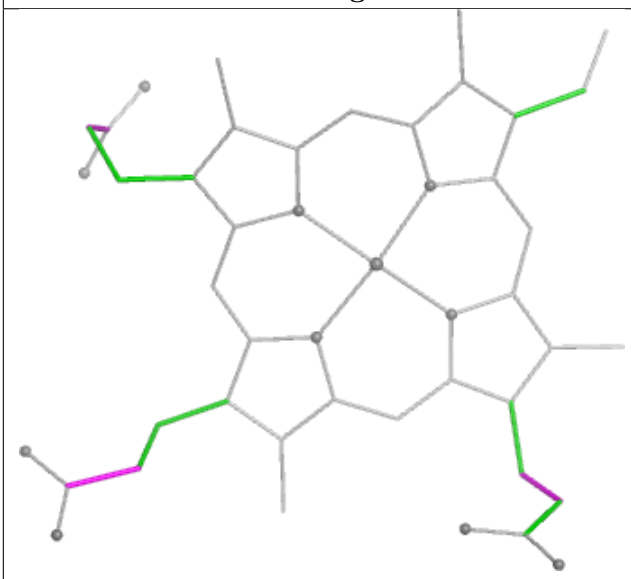
Ligand VOV B 303 (B)



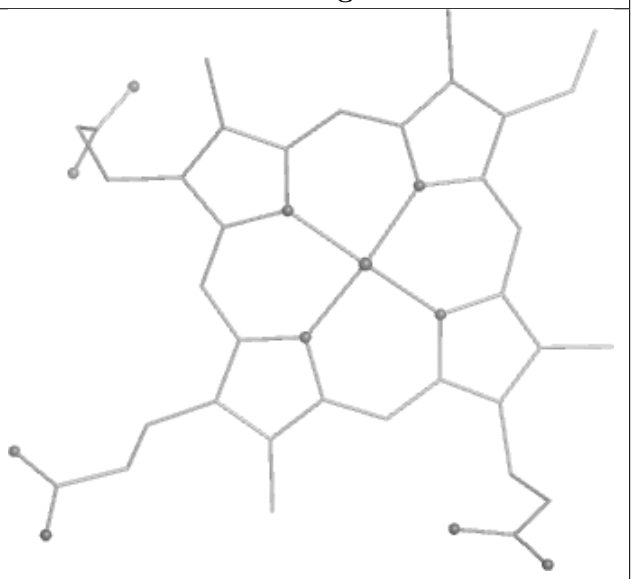
Bond lengths



Bond angles

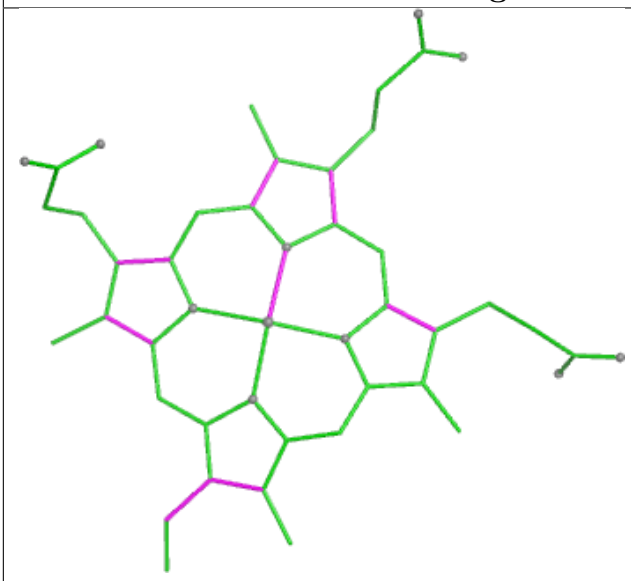


Torsions

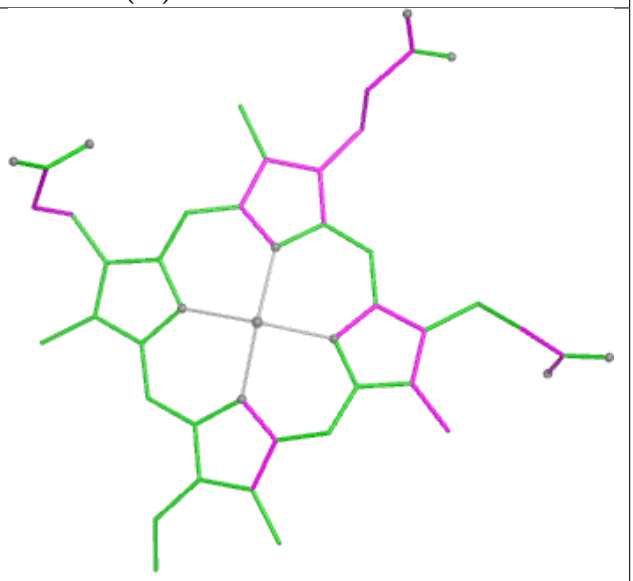


Rings

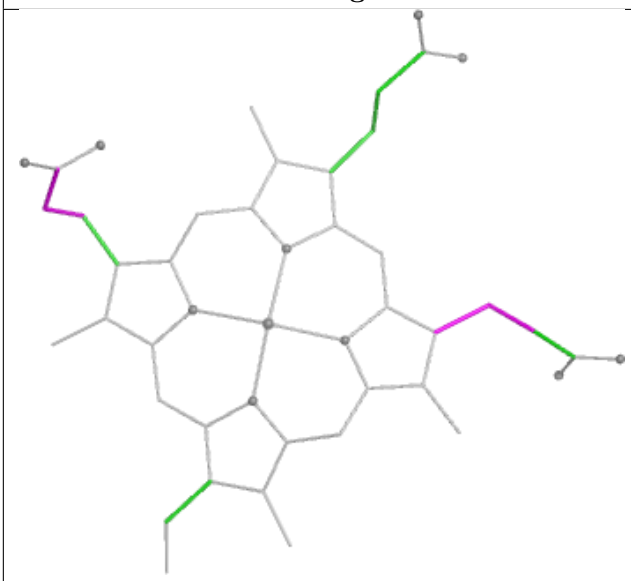
Ligand VOV C 302 (B)



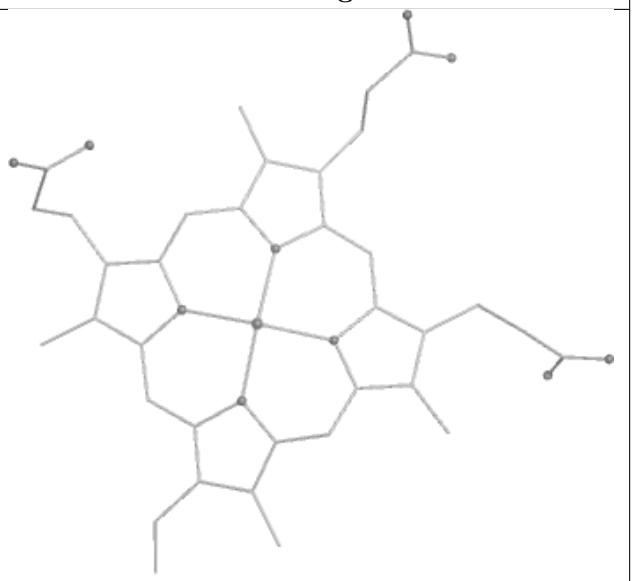
Bond lengths



Bond angles

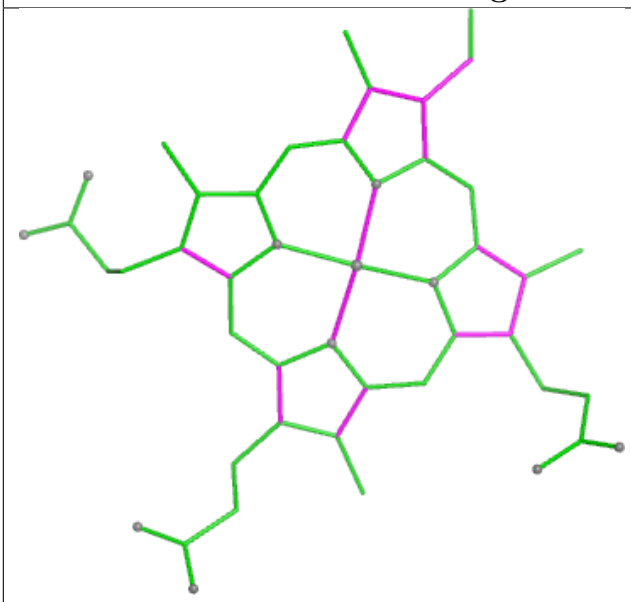


Torsions

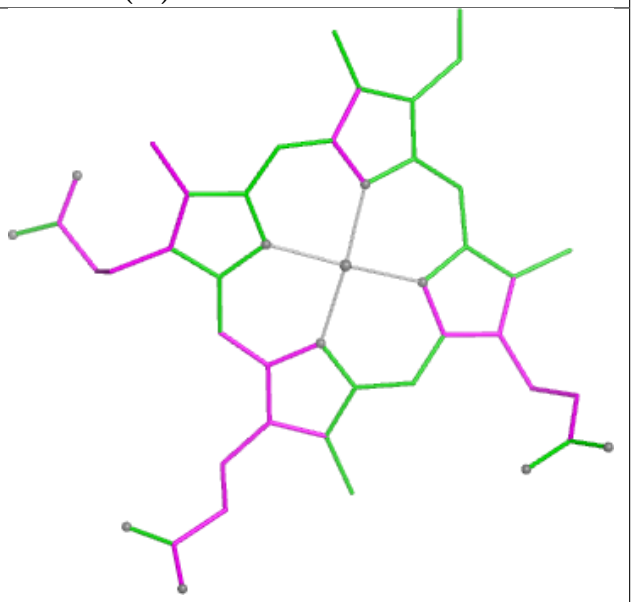


Rings

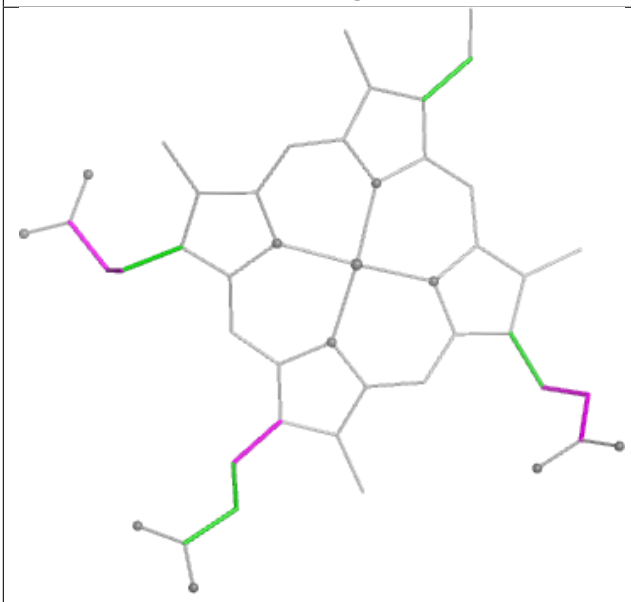
Ligand VOV E 302 (B)



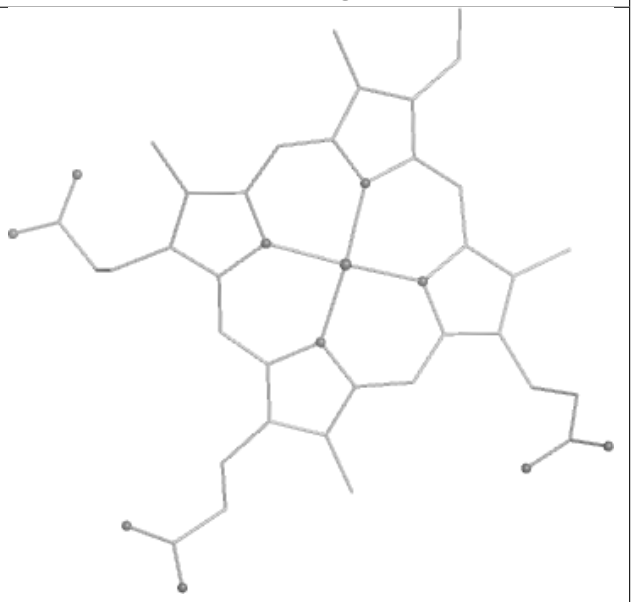
Bond lengths



Bond angles

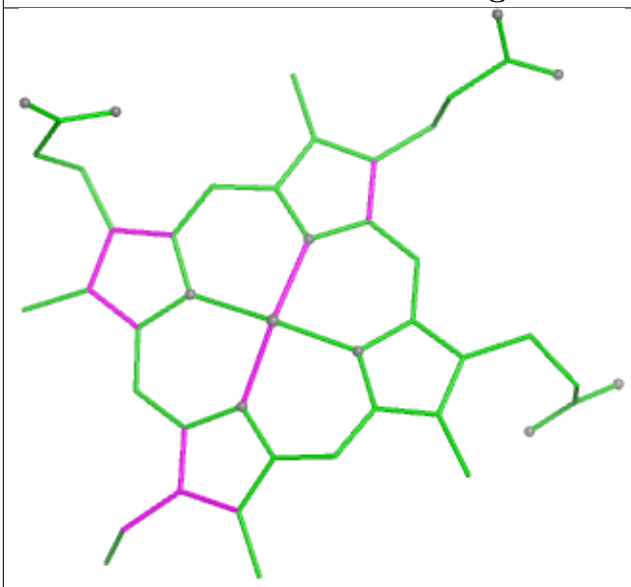


Torsions

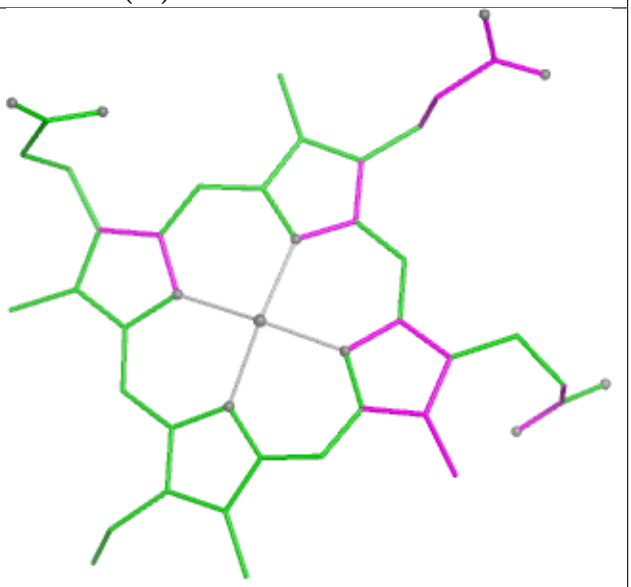


Rings

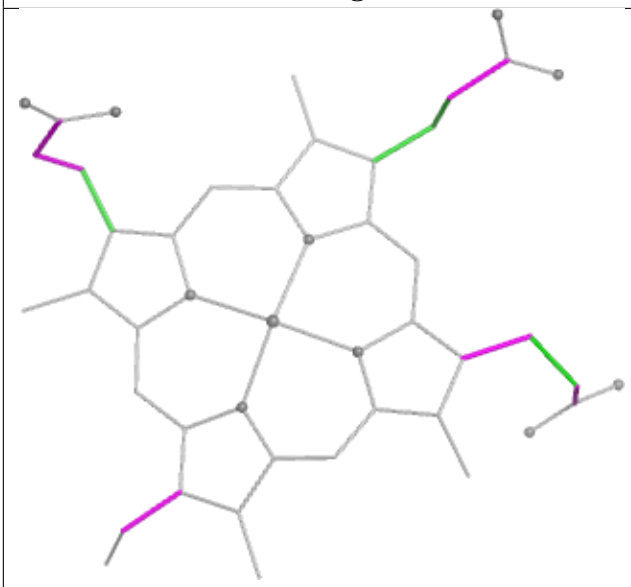
Ligand VOV A 303 (B)



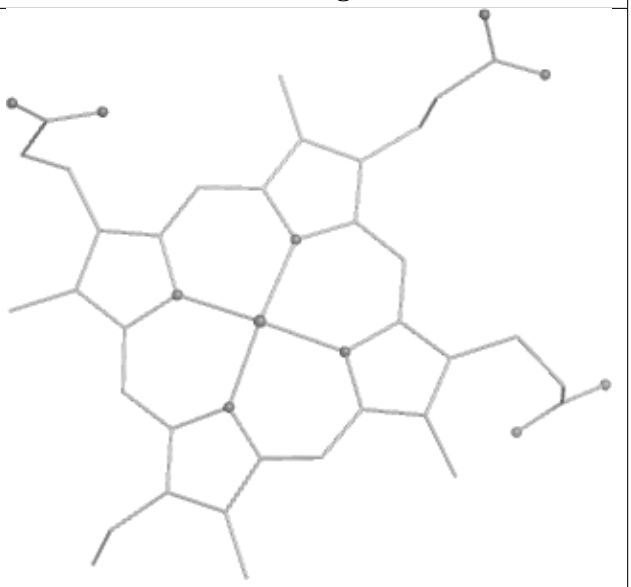
Bond lengths



Bond angles

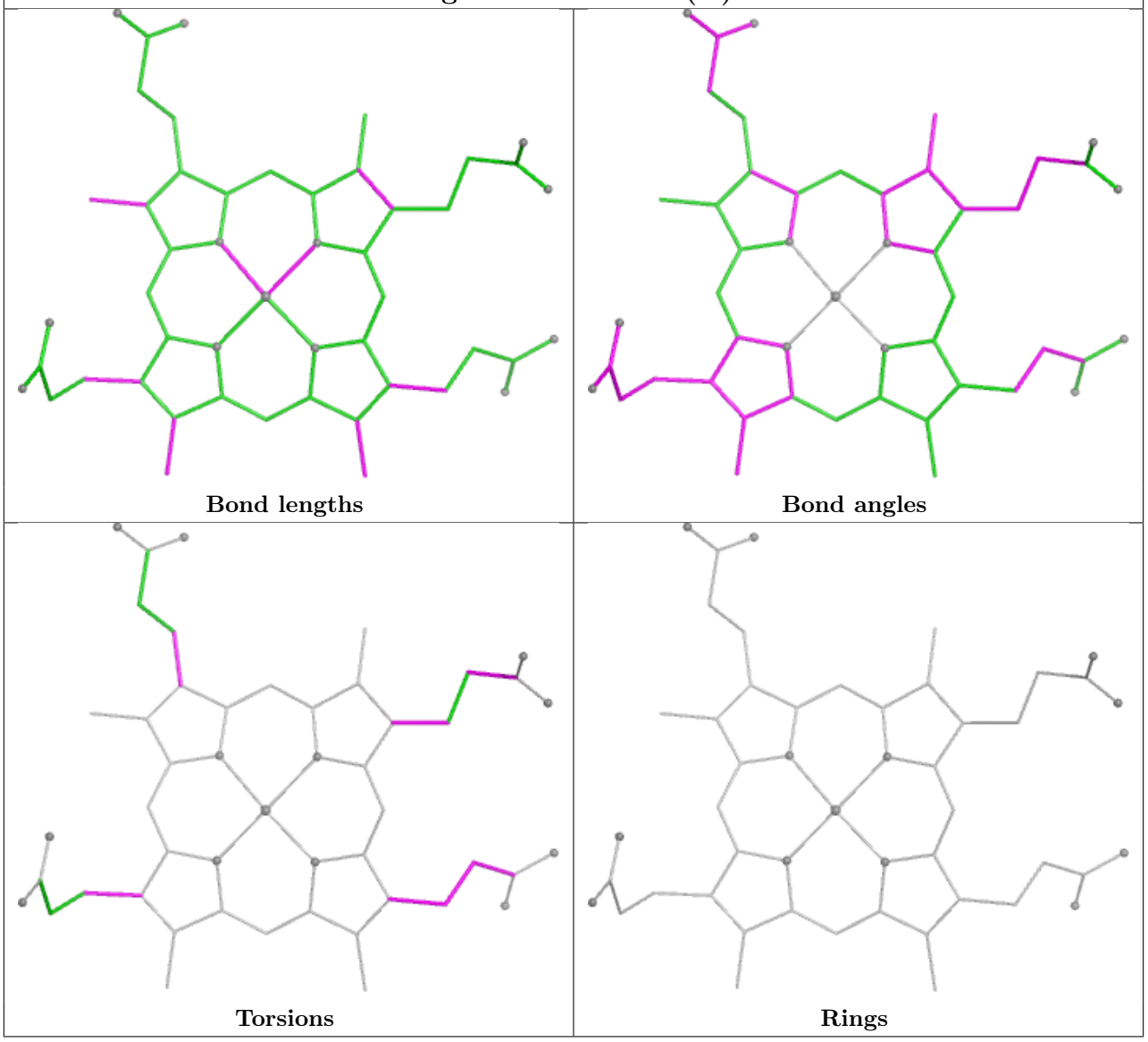


Torsions



Rings

Ligand FEC E 301 (A)



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	248/250 (99%)	-0.02	10 (4%) 42 46	25, 40, 70, 158	0
1	B	233/250 (93%)	-0.07	4 (1%) 69 73	24, 38, 69, 137	0
1	C	237/250 (94%)	-0.04	10 (4%) 40 45	23, 37, 82, 171	0
1	D	250/250 (100%)	-0.17	7 (2%) 55 59	22, 35, 63, 204	0
1	E	235/250 (94%)	-0.09	6 (2%) 57 61	24, 37, 82, 125	0
All	All	1203/1250 (96%)	-0.08	37 (3%) 51 55	22, 37, 75, 204	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	120	GLY	5.6
1	D	119	ALA	4.2
1	E	113	TYR	4.1
1	D	121	GLY	4.0
1	C	5	VAL	3.9
1	B	111	SER	3.8
1	C	113	TYR	3.7
1	C	128	LYS	3.6
1	E	125	TYR	3.6
1	C	3	GLU	3.3
1	C	4	ALA	3.3
1	C	129	GLY	3.2
1	A	4	ALA	3.2
1	A	251	ILE	3.2
1	B	125	TYR	2.9
1	E	111	SER	2.8
1	D	2	ASN	2.7
1	A	118	MET	2.6
1	A	121	GLY	2.6
1	D	251	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	120	GLY	2.5
1	C	29	ASN	2.4
1	E	243	GLU	2.4
1	A	246	SER	2.4
1	E	251	ILE	2.4
1	D	118	MET	2.3
1	C	126	GLN	2.3
1	B	6	LYS	2.3
1	B	8	LEU	2.2
1	D	117	HIS	2.2
1	E	246	SER	2.2
1	C	6	LYS	2.1
1	C	183	GLY	2.1
1	A	122	ASP	2.1
1	A	176	LEU	2.0
1	A	247	LYS	2.0
1	A	119	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no 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
4	VOV	C	302[B]	46/46	0.78	0.26	49,65,79,82	77
5	MPD	B	304	8/8	0.80	0.18	62,75,89,89	0
3	FEC	C	301[A]	49/49	0.83	0.22	48,65,79,80	81
4	VOV	D	302[B]	46/46	0.84	0.21	34,44,73,77	77
3	FEC	B	302[A]	49/49	0.86	0.20	54,61,76,77	81
3	FEC	E	301[A]	49/49	0.86	0.19	53,65,78,82	81

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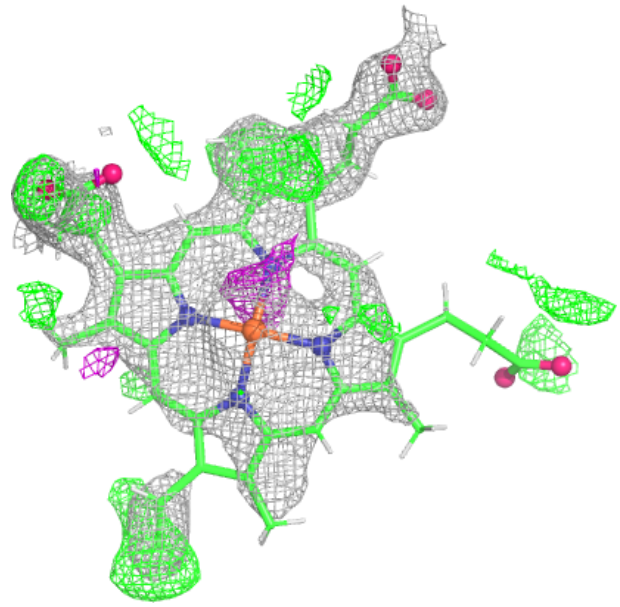
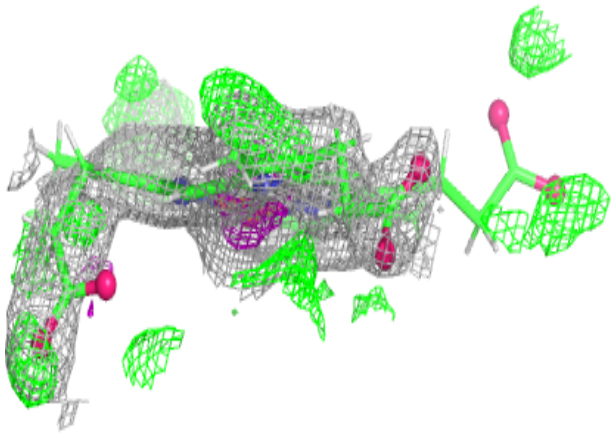
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	VOV	B	303[B]	46/46	0.86	0.19	53,60,76,77	77
5	MPD	D	303	8/8	0.86	0.15	62,75,96,96	0
4	VOV	E	302[B]	46/46	0.87	0.19	53,62,77,80	77
3	FEC	A	302[A]	49/49	0.88	0.18	36,49,62,65	81
5	MPD	A	304	8/8	0.88	0.18	54,72,91,109	0
5	MPD	E	303	8/8	0.90	0.14	56,72,87,87	0
4	VOV	A	303[B]	46/46	0.91	0.15	35,48,64,68	77
3	FEC	D	301[A]	49/49	0.93	0.14	34,45,65,70	81
2	NA	D	304	1/1	0.99	0.04	22,22,22,22	0
2	NA	A	301	1/1	0.99	0.03	25,25,25,25	0
2	NA	A	305	1/1	0.99	0.04	26,26,26,26	0
2	NA	B	301	1/1	0.99	0.03	27,27,27,27	0
2	NA	C	303	1/1	0.99	0.02	24,24,24,24	0

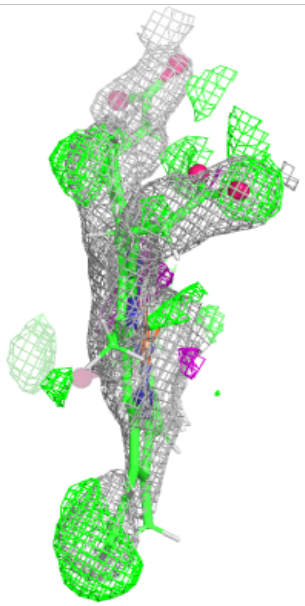
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around VOV C 302 (B):

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

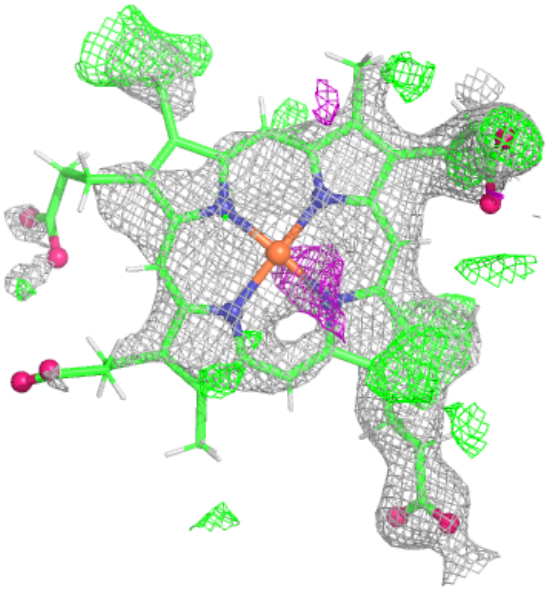


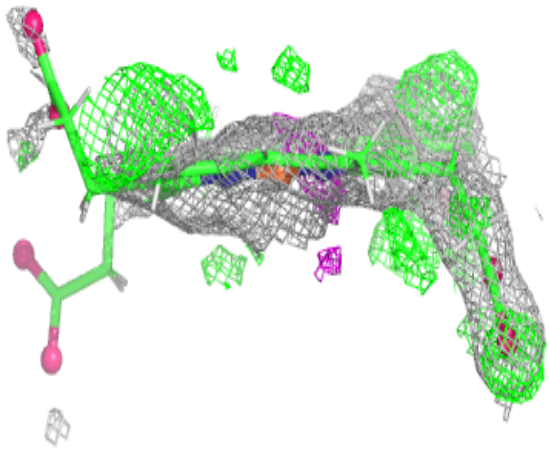


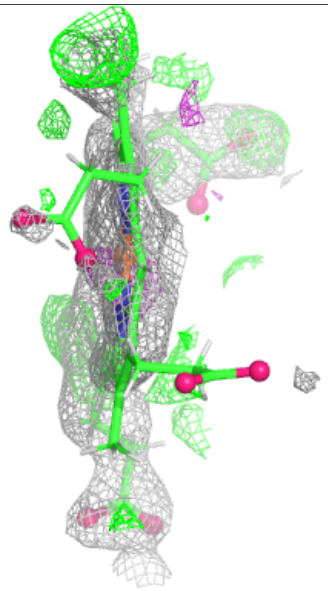


Electron density around FEC C 301 (A):

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

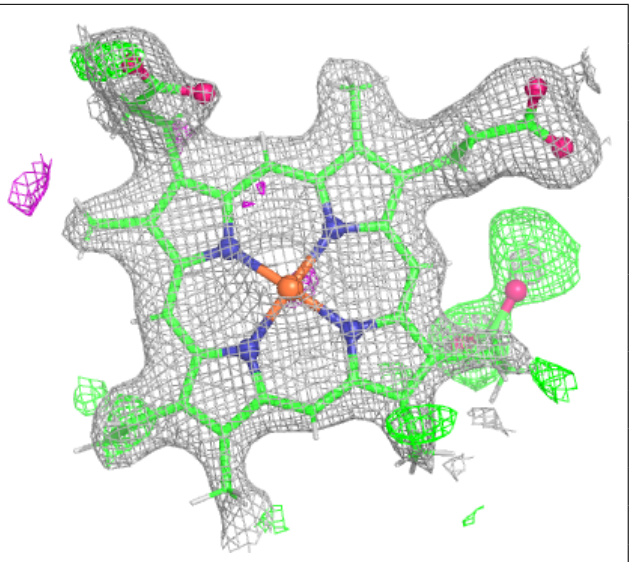


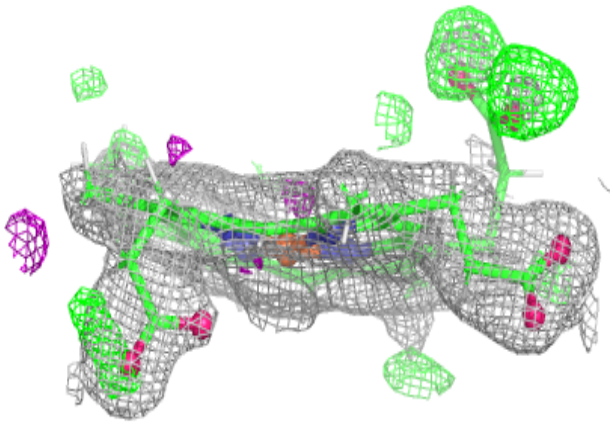


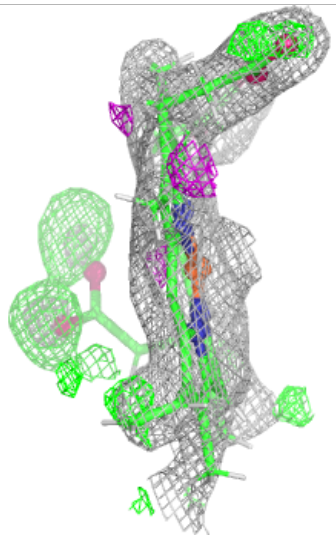


Electron density around VOV D 302 (B):

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

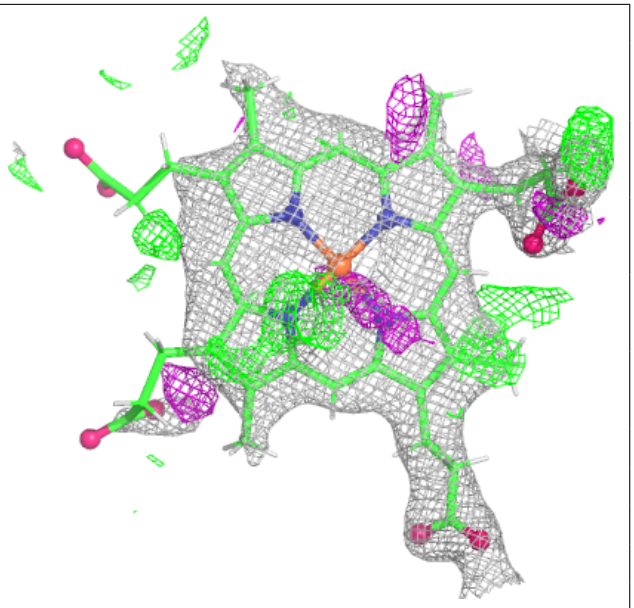


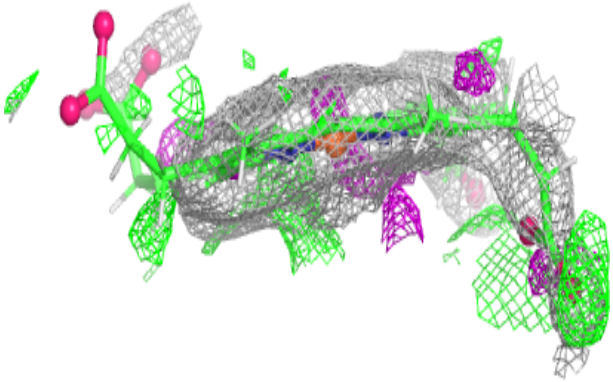


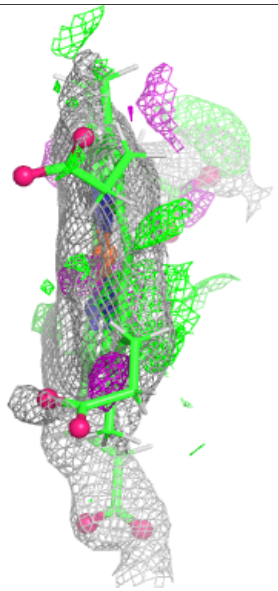


Electron density around FEC B 302 (A):

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

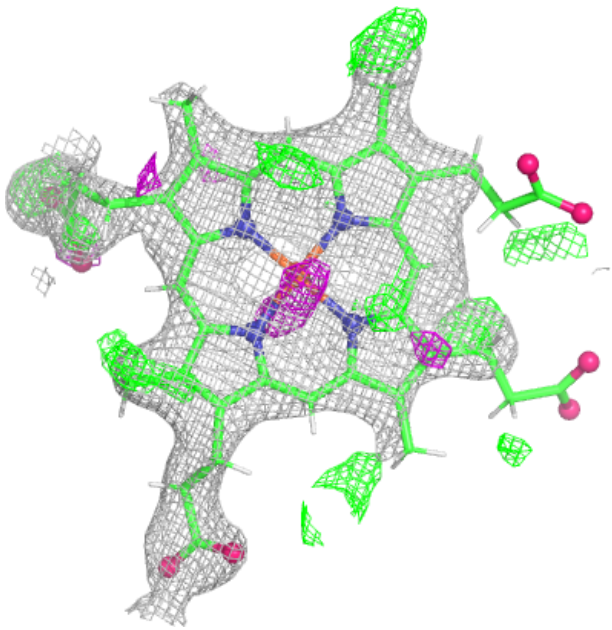


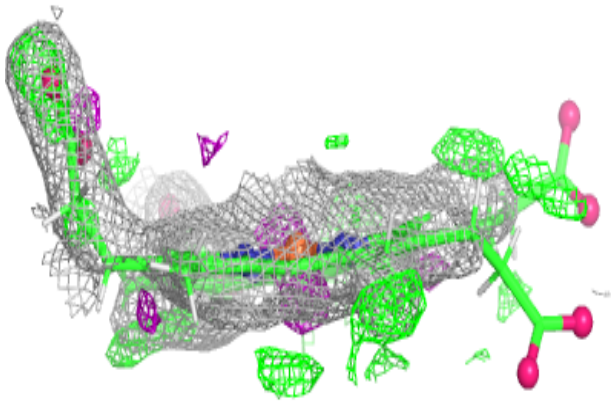


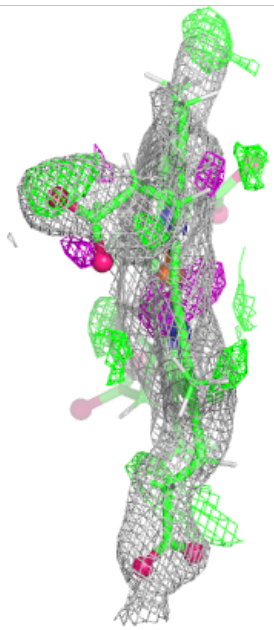


Electron density around FEC E 301 (A):

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

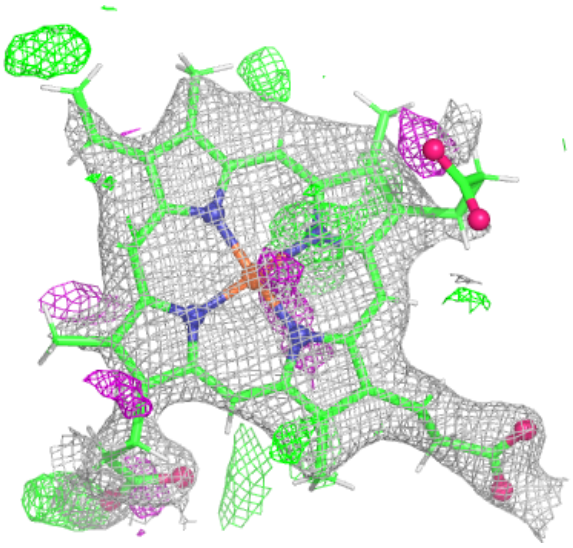


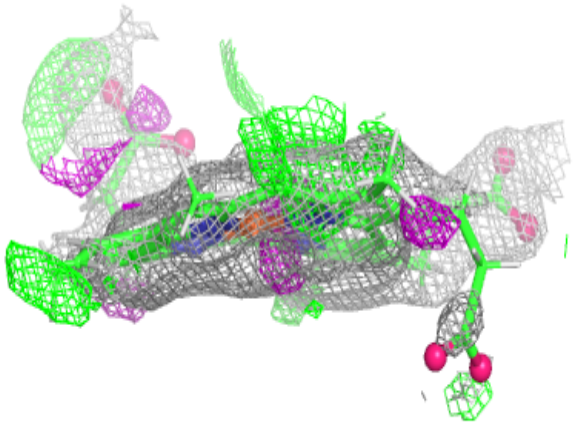


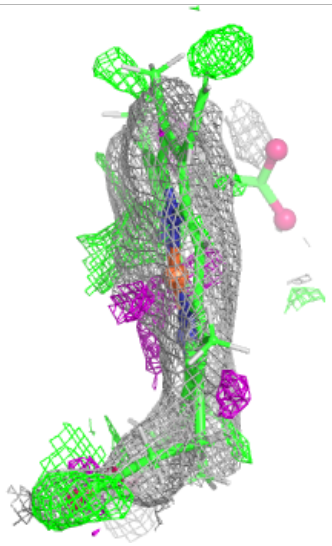


Electron density around VOV B 303 (B):

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

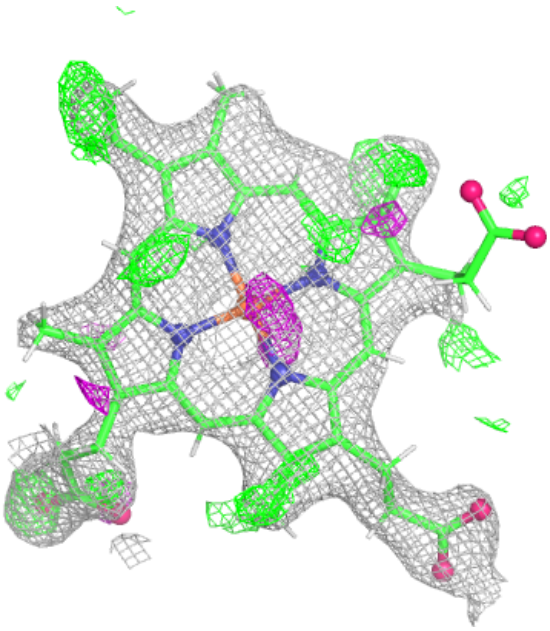


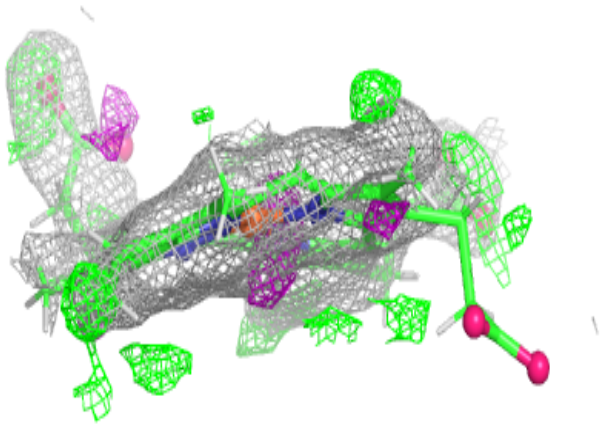


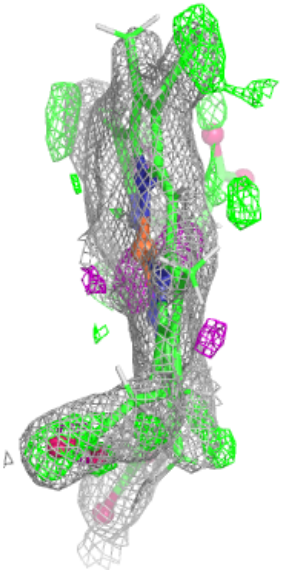


Electron density around VOV E 302 (B):

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

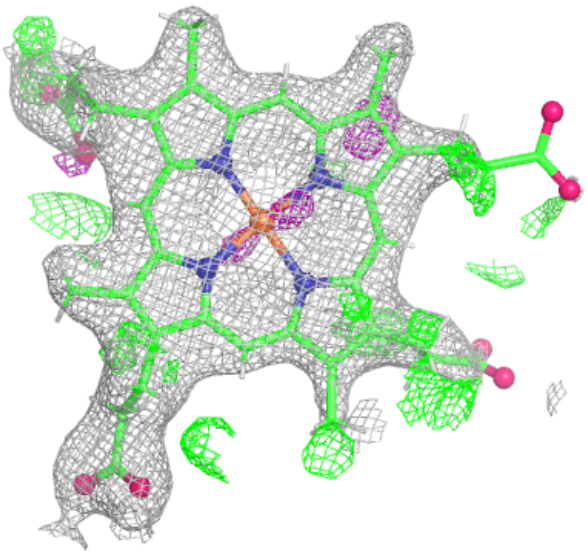


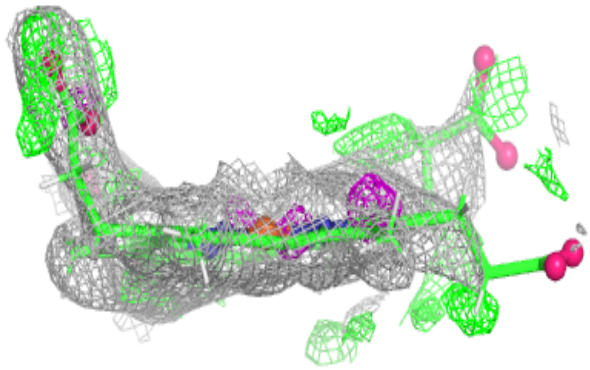


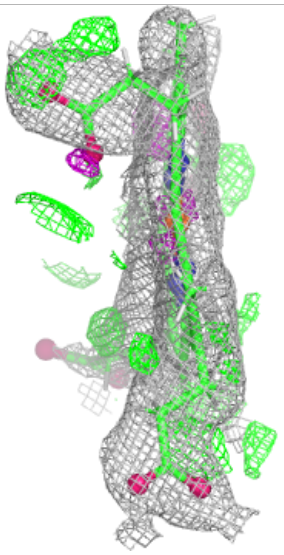


Electron density around FEC A 302 (A):

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

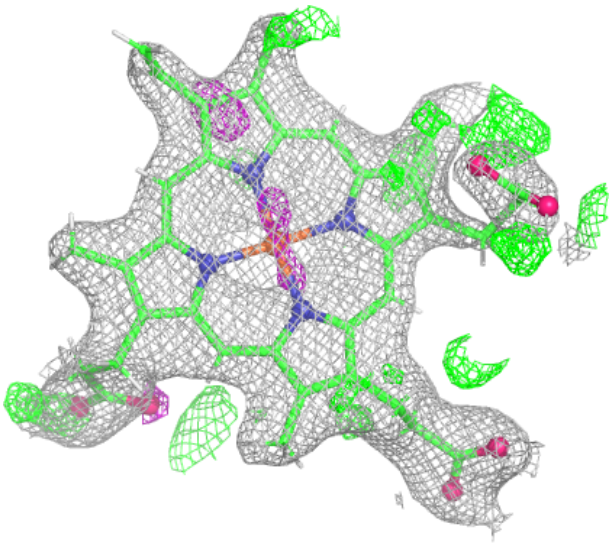


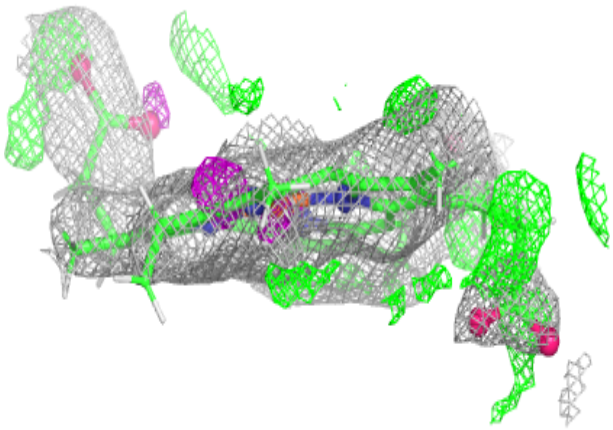


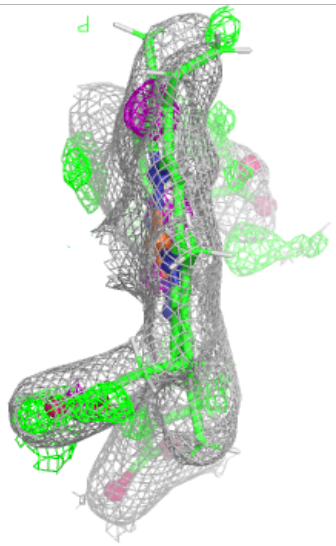


Electron density around VOV A 303 (B):

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

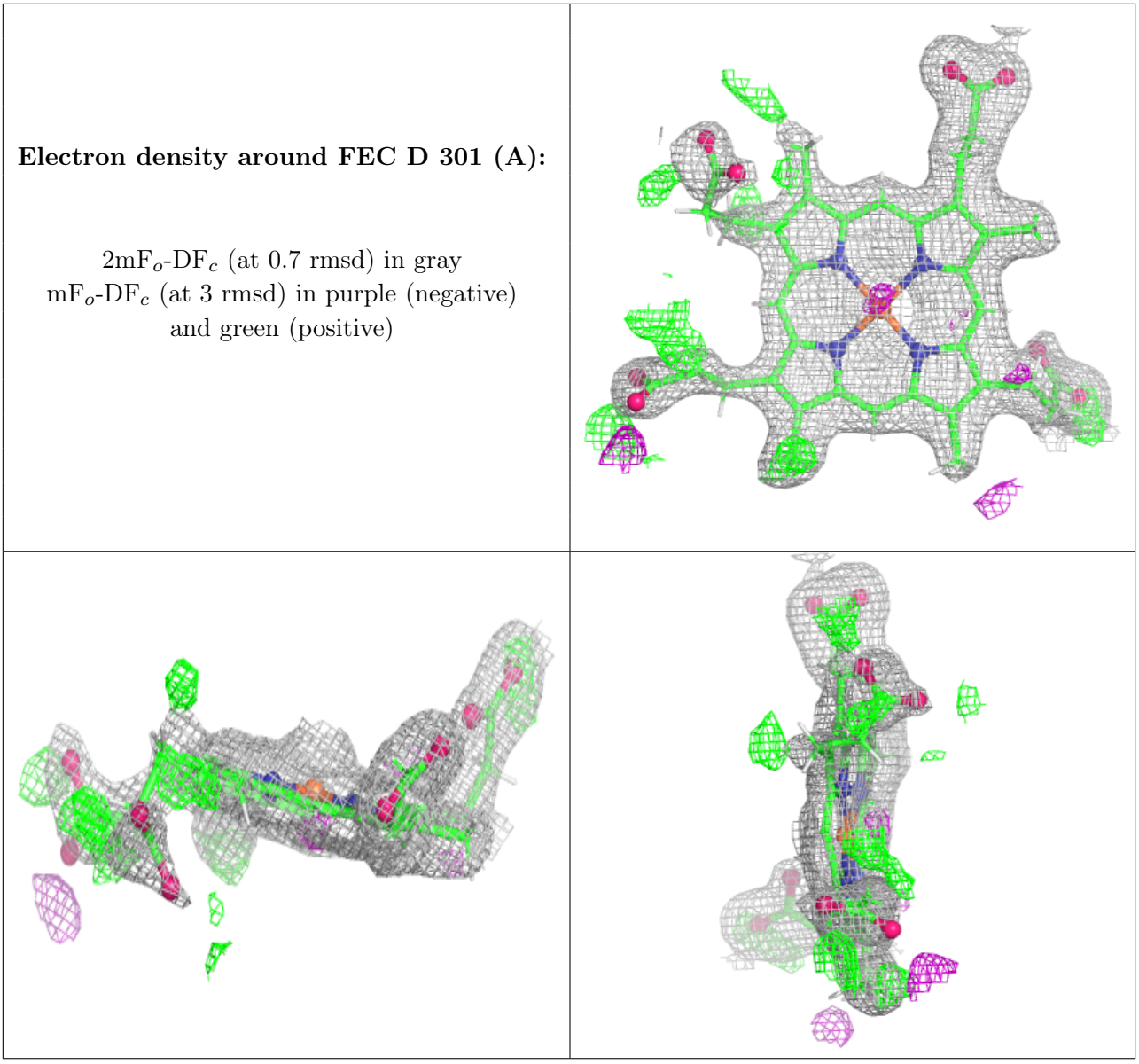






Electron density around FEC D 301 (A):

$2mF_o$-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.