Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2026 – 02:12 PM EDT

PDB ID	:	9MIQ / pdb_00009miq
Title	:	Wild-type Coproheme Decarboxylase from Streptomyces Coelicolor in complex with Monovinyl, Monopropionate Deuteroheme
Authors	:	Carriuolo, A.J.; Lanzilotta, W.N.
Deposited on	:	2024-12-13
Resolution	:	2.50 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:

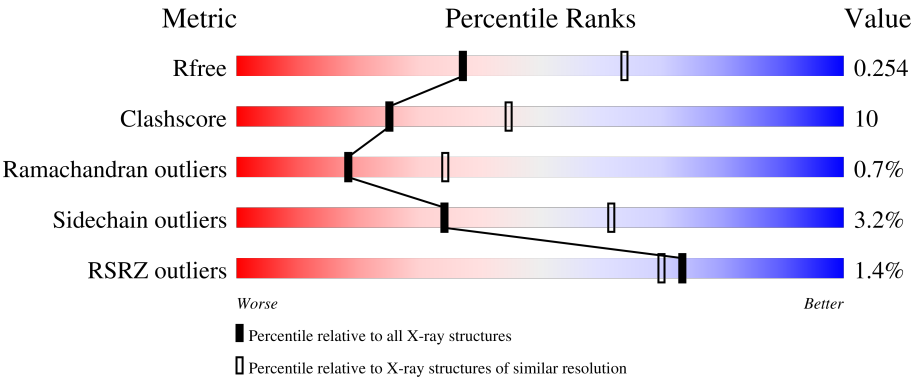
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 <=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	243	3% 64% 26% • 9%
1	B	243	74% 17% • 9%
1	C	243	% 68% 21% • 9%
1	D	243	76% 14% • 9%
1	E	243	% 75% 14% • 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	243	2% 71% 19% • 9%
1	G	243	68% 21% • 9%
1	H	243	2% 67% 23% • 9%
1	I	243	3% 65% 23% • 9%
1	J	243	% 75% 14% • 9%

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
2	VOV	A	301	X	-	-	-
2	VOV	B	301	X	-	-	-
2	VOV	C	301	X	-	-	-
2	VOV	D	301	X	-	-	-
2	VOV	E	301	X	-	-	-
2	VOV	F	301	X	-	-	-
2	VOV	G	301	X	-	-	-
2	VOV	H	301	X	-	-	-
2	VOV	I	301	X	-	-	-
2	VOV	J	301	X	-	-	-

2 Entry composition (i)

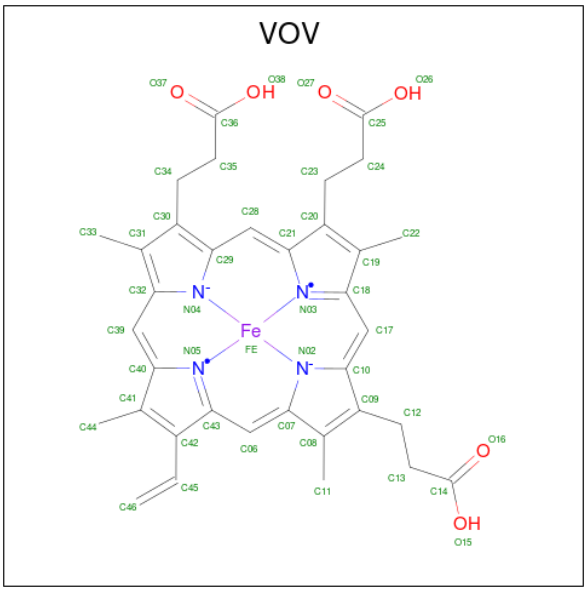
There are 3 unique types of molecules in this entry. The entry contains 18777 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Coproheme decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1827	1161	329	332	5			
1	B	222	Total	C	N	O	S	0	0	0
			1835	1165	330	335	5			
1	C	221	Total	C	N	O	S	0	0	0
			1827	1161	329	332	5			
1	D	222	Total	C	N	O	S	0	0	0
			1835	1165	330	335	5			
1	E	218	Total	C	N	O	S	0	0	0
			1802	1146	325	326	5			
1	F	221	Total	C	N	O	S	0	0	0
			1827	1161	329	332	5			
1	G	222	Total	C	N	O	S	0	0	0
			1835	1165	330	335	5			
1	H	221	Total	C	N	O	S	0	0	0
			1830	1162	329	334	5			
1	I	221	Total	C	N	O	S	0	0	0
			1827	1161	329	332	5			
1	J	222	Total	C	N	O	S	0	0	0
			1835	1165	330	335	5			

- Molecule 2 is harderoheme (III) (CCD ID: VOV) (formula: $C_{35}H_{34}FeN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			46	35	1	4	6		
2	B	1	Total	C	Fe	N	O	0	0
			46	35	1	4	6		
2	C	1	Total	C	Fe	N	O	0	0
			46	35	1	4	6		
2	D	1	Total	C	Fe	N	O	0	0
			46	35	1	4	6		
2	E	1	Total	C	Fe	N	O	0	0
			46	35	1	4	6		
2	F	1	Total	C	Fe	N	O	0	0
			46	35	1	4	6		
2	G	1	Total	C	Fe	N	O	0	0
			46	35	1	4	6		
2	H	1	Total	C	Fe	N	O	0	0
			46	35	1	4	6		
2	I	1	Total	C	Fe	N	O	0	0
			46	35	1	4	6		
2	J	1	Total	C	Fe	N	O	0	0
			46	35	1	4	6		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		
3	B	3	Total	O	0	0
			3	3		

Continued on next page...

Continued from previous page...

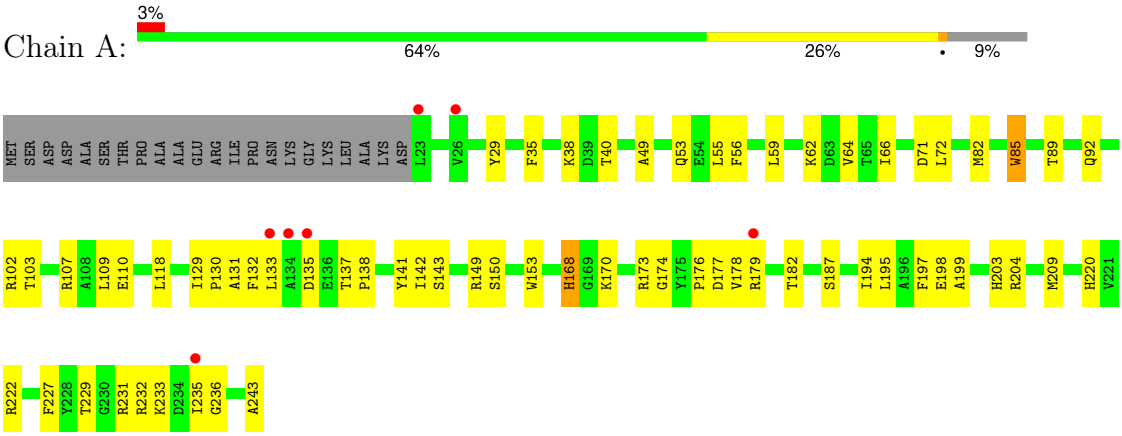
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	5	Total O 5 5	0	0
3	D	6	Total O 6 6	0	0
3	E	3	Total O 3 3	0	0
3	F	7	Total O 7 7	0	0
3	G	1	Total O 1 1	0	0
3	H	5	Total O 5 5	0	0
3	I	1	Total O 1 1	0	0
3	J	3	Total O 3 3	0	0

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.

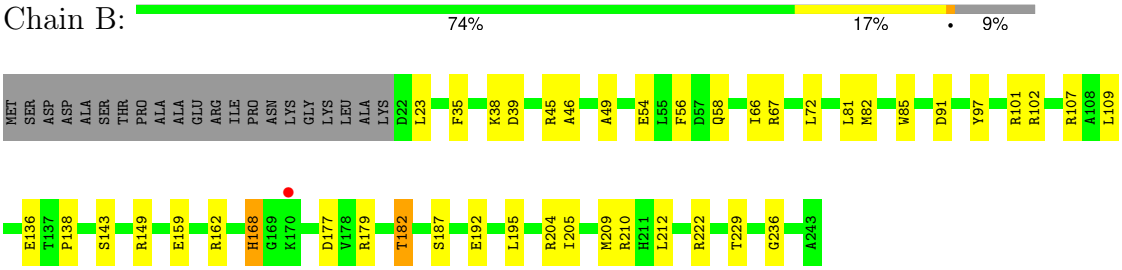
• Molecule 1: Coproheme decarboxylase

Chain A:



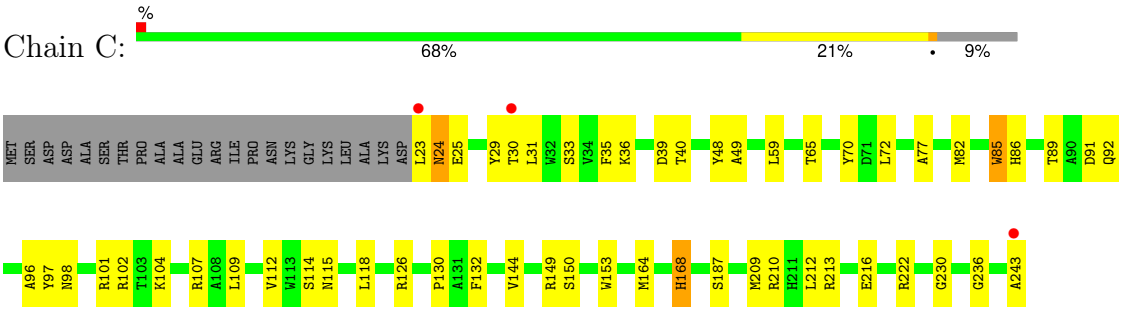
• Molecule 1: Coproheme decarboxylase

Chain B:



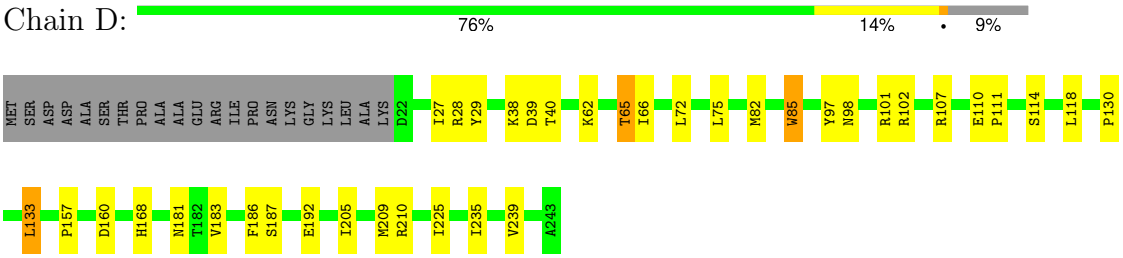
• Molecule 1: Coproheme decarboxylase

Chain C:



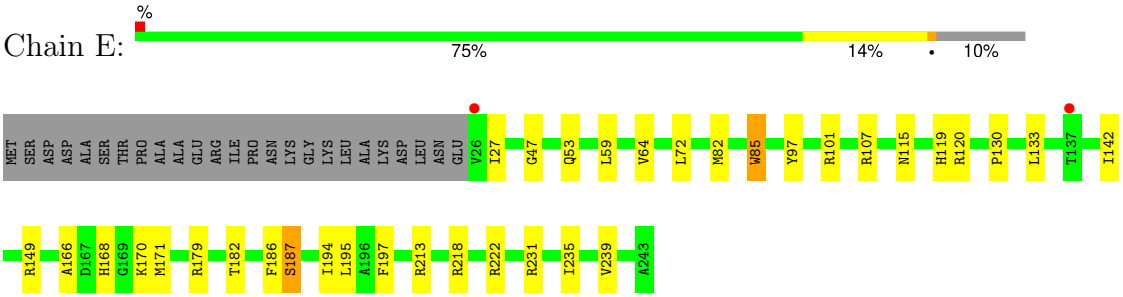
• Molecule 1: Coproheme decarboxylase

Chain D:



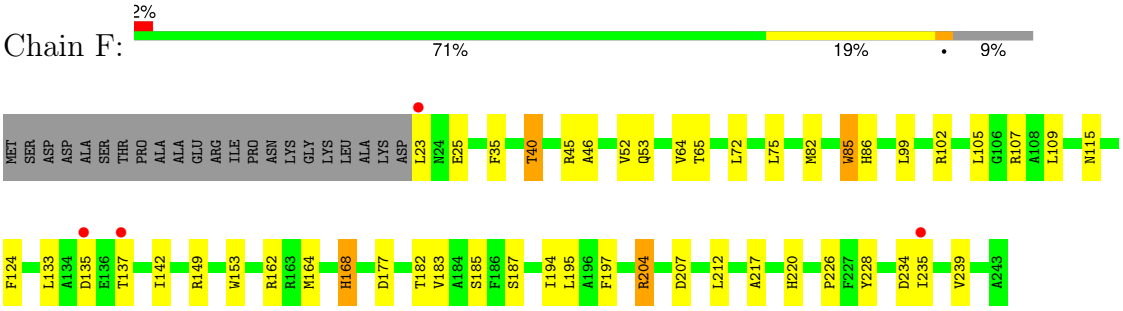
• Molecule 1: Coproheme decarboxylase

Chain E:



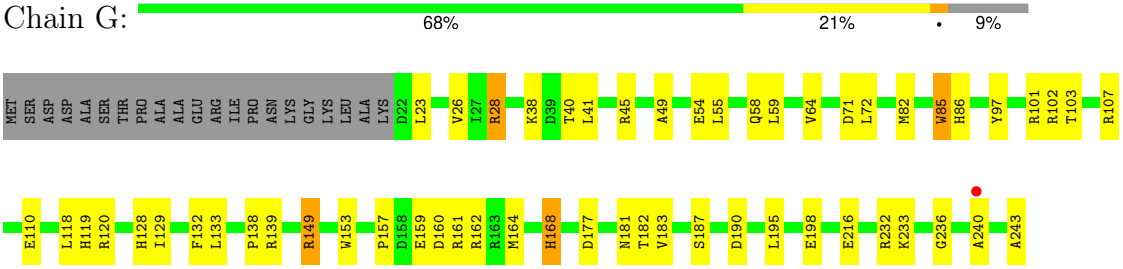
• Molecule 1: Coproheme decarboxylase

Chain F:



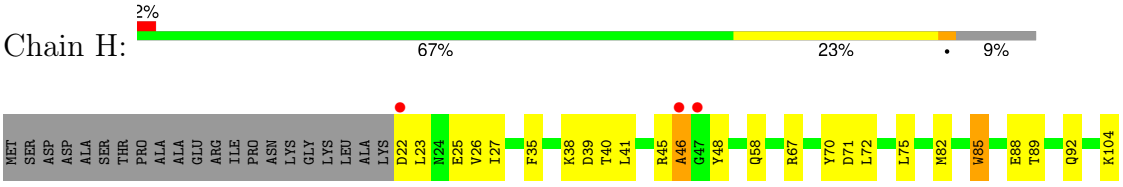
• Molecule 1: Coproheme decarboxylase

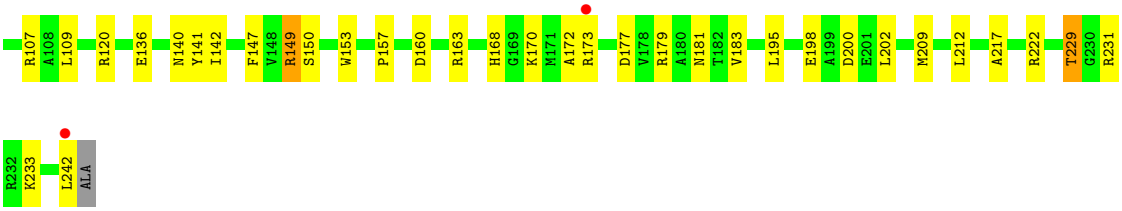
Chain G:



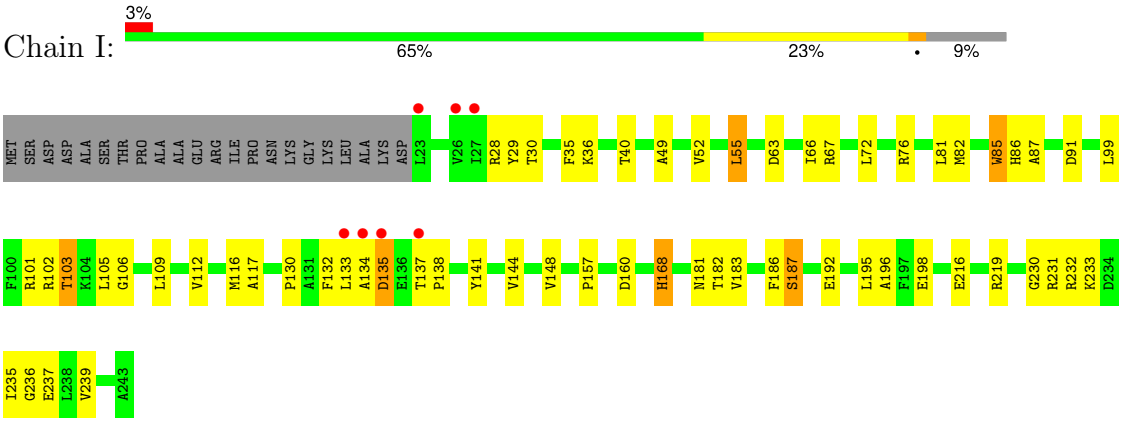
• Molecule 1: Coproheme decarboxylase

Chain H:

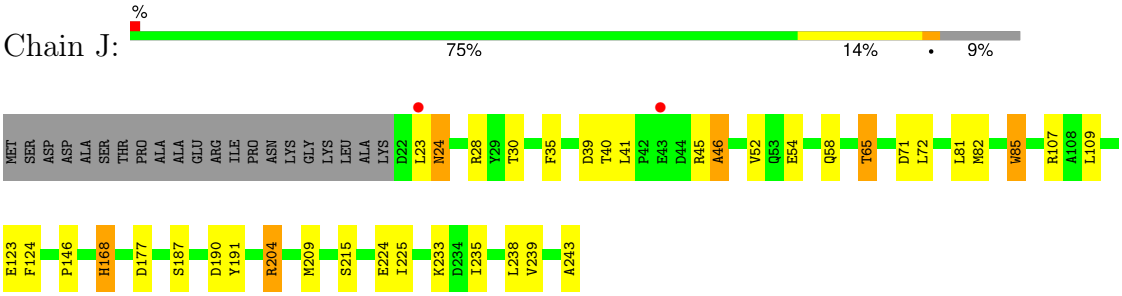




• Molecule 1: Coproheme decarboxylase



• Molecule 1: Coproheme decarboxylase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	184.71Å 184.71Å 241.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.00 – 2.50 42.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (42.00-2.50) 93.2 (42.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.70 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.21.1_5286: ???)	Depositor
R, R_{free}	0.209 , 0.254 0.208 , 0.254	Depositor DCC
R_{free} test set	2000 reflections (1.41%)	wwPDB-VP
Wilson B-factor (Å^2)	54.2	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 33.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18777	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% 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: VOV

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	0.47	0/1874	0.65	0/2541
1	B	0.51	0/1882	0.66	1/2552 (0.0%)
1	C	0.50	0/1874	0.69	0/2541
1	D	0.51	0/1882	0.67	0/2552
1	E	0.48	0/1849	0.66	0/2507
1	F	0.46	0/1874	0.62	0/2541
1	G	0.47	0/1882	0.65	0/2552
1	H	0.47	0/1877	0.67	0/2545
1	I	0.47	0/1874	0.66	0/2541
1	J	0.48	0/1882	0.70	1/2552 (0.0%)
All	All	0.48	0/18750	0.66	2/25424 (0.0%)

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	E	0	1
1	G	0	1
1	H	0	1
1	J	0	2
All	All	0	5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	24	ASN	N-CA-C	-6.23	97.53	110.80
1	B	39	ASP	CB-CA-C	-5.88	109.24	117.23

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	47	GLY	Peptide
1	G	28	ARG	Sidechain
1	H	149	ARG	Sidechain
1	J	204	ARG	Sidechain
1	J	23	LEU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1827	0	1770	54	0
1	B	1835	0	1774	25	0
1	C	1827	0	1770	51	0
1	D	1835	0	1774	27	0
1	E	1802	0	1747	23	0
1	F	1827	0	1768	36	0
1	G	1835	0	1773	39	0
1	H	1830	0	1769	48	0
1	I	1827	0	1770	53	0
1	J	1835	0	1774	36	0
2	A	46	0	0	2	0
2	B	46	0	0	1	0
2	C	46	0	0	3	0
2	D	46	0	0	0	0
2	E	46	0	0	1	0
2	F	46	0	0	2	0
2	G	46	0	0	1	0
2	H	46	0	0	2	0
2	I	46	0	0	1	0
2	J	46	0	0	3	0
3	A	3	0	0	1	0
3	B	3	0	0	0	0
3	C	5	0	0	0	0
3	D	6	0	0	0	0
3	E	3	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	7	0	0	0	0
3	G	1	0	0	0	0
3	H	5	0	0	0	0
3	I	1	0	0	0	0
3	J	3	0	0	0	0
All	All	18777	0	17689	353	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 10.

All (353) 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:I:40:THR:HG21	1:J:107:ARG:HH12	1.15	1.11
1:H:67:ARG:NH1	1:H:198:GLU:OE2	2.08	0.87
1:G:190:ASP:HB3	1:J:225:ILE:HD11	1.59	0.84
1:I:52:VAL:HG23	1:I:103:THR:HG21	1.58	0.83
1:I:40:THR:HG21	1:J:107:ARG:NH1	1.93	0.83
1:B:182:THR:HB	1:B:195:LEU:HD22	1.63	0.81
1:I:103:THR:HG22	1:I:105:LEU:H	1.47	0.80
1:H:157:PRO:HG2	1:H:160:ASP:OD2	1.83	0.78
1:H:229:THR:HG21	1:I:187:SER:O	1.85	0.77
1:A:209:MET:HG3	1:C:187:SER:HB3	1.69	0.75
1:G:149:ARG:HD3	1:G:153:TRP:CD1	2.22	0.74
1:A:102:ARG:O	1:A:107:ARG:NH1	2.21	0.73
1:B:177:ASP:OD2	1:B:204:ARG:NH1	2.22	0.72
1:G:159:GLU:OE1	1:G:162:ARG:NH1	2.22	0.72
1:G:187:SER:HB3	1:J:209:MET:HG3	1.71	0.72
1:C:164:MET:HE2	1:C:216:GLU:HB3	1.71	0.72
1:B:168:HIS:HE1	2:B:301:VOV:N02	1.88	0.71
1:C:209:MET:HG3	1:D:187:SER:HB3	1.71	0.71
1:I:55:LEU:HD11	1:I:99:LEU:HB3	1.71	0.71
1:A:235:ILE:HD12	1:A:235:ILE:H	1.56	0.71
1:F:23:LEU:N	1:F:25:GLU:OE2	2.23	0.71
1:E:179:ARG:NH1	3:E:401:HOH:O	2.24	0.70
1:E:149:ARG:O	1:E:222:ARG:HD3	1.91	0.69
1:D:181:ASN:O	1:D:183:VAL:HG23	1.92	0.69
1:I:67:ARG:NH1	1:I:198:GLU:OE2	2.27	0.68
1:H:67:ARG:HH12	1:H:198:GLU:CD	2.02	0.68
1:F:177:ASP:OD2	1:F:204:ARG:HG2	1.93	0.67
1:D:40:THR:HG21	1:E:107:ARG:HH12	1.59	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:120:ARG:HE	1:H:120:ARG:HA	1.59	0.67
1:B:72:LEU:HD11	1:B:82:MET:HB2	1.78	0.65
1:F:102:ARG:O	1:F:107:ARG:NH1	2.29	0.65
1:C:30:THR:HG23	1:C:132:PHE:CE2	2.31	0.65
1:I:168:HIS:HE1	2:I:301:VOV:N02	1.94	0.65
1:G:28:ARG:HD2	1:G:86:HIS:ND1	2.12	0.64
1:E:182:THR:HG22	1:E:195:LEU:HG	1.79	0.64
1:C:168:HIS:HE1	2:C:301:VOV:N02	1.97	0.63
1:A:49:ALA:HB1	1:A:236:GLY:HA2	1.80	0.62
1:D:40:THR:HG21	1:E:107:ARG:NH1	2.15	0.62
1:H:209:MET:HG3	1:I:187:SER:HB2	1.82	0.62
1:F:207:ASP:OD2	1:H:120:ARG:NH1	2.33	0.61
1:G:157:PRO:HG2	1:G:160:ASP:OD2	2.00	0.61
1:H:141:TYR:CE1	1:H:231:ARG:HG2	2.34	0.61
1:J:177:ASP:OD2	1:J:204:ARG:HG3	2.01	0.61
1:C:65:THR:OG1	1:C:86:HIS:NE2	2.34	0.61
1:H:89:THR:H	1:H:92:GLN:NE2	1.98	0.61
1:F:53:GLN:OE1	1:F:235:ILE:HD13	2.01	0.60
1:D:27:ILE:HG23	1:D:118:LEU:HD11	1.83	0.60
1:B:149:ARG:O	1:B:222:ARG:HD3	2.01	0.59
1:D:29:TYR:CE1	1:D:118:LEU:HD13	2.38	0.59
1:F:164:MET:HE1	1:F:220:HIS:ND1	2.17	0.59
1:G:97:TYR:CE1	1:G:101:ARG:HD3	2.38	0.59
1:B:102:ARG:O	1:B:107:ARG:NH1	2.35	0.59
1:G:45:ARG:HH11	1:G:240:ALA:HA	1.67	0.59
1:A:53:GLN:O	1:A:53:GLN:NE2	2.35	0.59
1:A:56:PHE:CE2	1:A:66:ILE:HG21	2.38	0.59
1:I:235:ILE:O	1:I:239:VAL:HG23	2.03	0.59
1:J:168:HIS:CE1	2:J:301:VOV:N02	2.71	0.59
1:H:45:ARG:HH12	1:I:102:ARG:HH21	1.51	0.58
1:H:231:ARG:HG3	1:I:91:ASP:OD2	2.03	0.58
1:A:170:LYS:HG3	1:A:173:ARG:NH1	2.19	0.58
1:D:102:ARG:O	1:D:107:ARG:NH1	2.35	0.58
1:I:103:THR:HG22	1:I:105:LEU:N	2.16	0.58
1:D:38:LYS:HG2	1:D:110:GLU:HG2	1.86	0.57
1:A:38:LYS:HG2	1:A:110:GLU:HG2	1.86	0.57
1:H:39:ASP:O	1:I:101:ARG:NH2	2.37	0.57
1:B:91:ASP:OD2	1:E:231:ARG:HD3	2.05	0.57
1:A:103:THR:O	1:A:107:ARG:HG3	2.05	0.57
1:G:118:LEU:HD23	1:G:120:ARG:HD3	1.86	0.57
1:H:88:GLU:H	1:H:92:GLN:HE22	1.53	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:LEU:C	1:C:25:GLU:H	2.13	0.56
1:I:130:PRO:HG3	1:I:183:VAL:HG12	1.86	0.56
1:F:23:LEU:HD12	1:F:133:LEU:HG	1.87	0.56
1:A:72:LEU:HD11	1:A:82:MET:HB2	1.87	0.56
1:C:48:TYR:CZ	1:C:104:LYS:HG2	2.41	0.56
1:I:117:ALA:CB	1:I:183:VAL:HG23	2.35	0.55
1:F:40:THR:HG21	1:H:107:ARG:HH12	1.71	0.55
1:C:97:TYR:CE1	1:C:101:ARG:HD2	2.42	0.55
1:A:40:THR:HG21	1:C:107:ARG:NH2	2.21	0.55
1:A:177:ASP:OD1	1:A:204:ARG:NH1	2.40	0.55
1:E:235:ILE:O	1:E:239:VAL:HG23	2.06	0.55
1:E:59:LEU:HB3	1:E:64:VAL:HB	1.88	0.55
1:A:130:PRO:HG2	1:A:133:LEU:HG	1.88	0.55
1:C:213:ARG:NH1	1:D:192:GLU:OE2	2.36	0.55
1:H:89:THR:H	1:H:92:GLN:HE21	1.54	0.55
1:A:71:ASP:HB2	1:A:233:LYS:HD3	1.89	0.54
1:C:30:THR:HG23	1:C:132:PHE:CZ	2.41	0.54
1:D:29:TYR:CZ	1:D:118:LEU:HD13	2.43	0.54
1:B:136:GLU:OE1	1:B:179:ARG:HD2	2.07	0.54
1:F:149:ARG:HD2	1:F:153:TRP:CE2	2.42	0.54
1:I:49:ALA:HB1	1:I:236:GLY:HA2	1.90	0.54
1:C:149:ARG:NE	2:C:301:VOV:O27	2.40	0.53
1:D:97:TYR:CE1	1:D:101:ARG:HD3	2.43	0.53
1:D:209:MET:HG3	1:E:187:SER:HB2	1.89	0.53
1:H:71:ASP:HB2	1:H:233:LYS:HD2	1.90	0.53
1:G:71:ASP:HB2	1:G:233:LYS:HD2	1.89	0.53
1:H:168:HIS:CE1	2:H:301:VOV:N02	2.77	0.53
1:I:52:VAL:CG2	1:I:103:THR:HG21	2.34	0.53
1:E:53:GLN:HG2	1:E:235:ILE:CG2	2.39	0.53
1:J:52:VAL:CG1	1:J:235:ILE:HD13	2.39	0.53
1:A:141:TYR:OH	1:C:91:ASP:OD1	2.24	0.53
1:E:72:LEU:HD11	1:E:82:MET:HB2	1.91	0.53
1:I:186:PHE:CE2	1:I:192:GLU:HB3	2.43	0.53
1:A:149:ARG:HD2	1:A:153:TRP:CD2	2.43	0.53
1:A:243:ALA:N	1:C:98:ASN:OD1	2.40	0.53
1:B:177:ASP:OD2	1:B:204:ARG:HG3	2.09	0.53
1:C:89:THR:OG1	1:C:92:GLN:HG3	2.08	0.53
1:D:130:PRO:HG2	1:D:133:LEU:HB2	1.91	0.53
1:J:28:ARG:HH21	1:J:65:THR:HG23	1.74	0.53
1:D:157:PRO:HG2	1:D:160:ASP:OD2	2.09	0.52
1:G:102:ARG:HH12	1:J:45:ARG:NH2	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:THR:HG22	3:A:401:HOH:O	2.10	0.52
1:A:170:LYS:HG3	1:A:173:ARG:HH12	1.74	0.52
1:C:30:THR:CG2	1:C:132:PHE:CE2	2.93	0.52
1:A:168:HIS:HE1	2:A:301:VOV:N02	2.08	0.52
1:J:72:LEU:HD11	1:J:82:MET:HB2	1.92	0.52
1:D:72:LEU:HD11	1:D:82:MET:HB2	1.91	0.52
1:I:85:TRP:CD1	1:I:85:TRP:H	2.28	0.52
1:C:29:TYR:CE1	1:C:118:LEU:HD13	2.45	0.52
1:G:138:PRO:HB2	1:G:232:ARG:HE	1.75	0.52
1:H:75:LEU:HG	1:I:116:MET:HE3	1.91	0.52
1:A:130:PRO:HB2	1:A:132:PHE:CD1	2.46	0.51
1:I:28:ARG:HD2	1:I:86:HIS:ND1	2.25	0.51
1:A:149:ARG:HD2	1:A:153:TRP:CG	2.45	0.51
1:A:150:SER:HB3	1:A:220:HIS:HA	1.91	0.51
1:G:59:LEU:HB3	1:G:64:VAL:HB	1.93	0.51
1:I:157:PRO:HG2	1:I:160:ASP:OD2	2.09	0.51
1:E:142:ILE:HA	1:E:197:PHE:O	2.10	0.51
1:G:54:GLU:HG2	1:G:58:GLN:HE21	1.75	0.51
1:I:216:GLU:O	1:I:219:ARG:HG3	2.11	0.51
1:J:54:GLU:OE2	1:J:54:GLU:HA	2.11	0.51
1:F:164:MET:CE	1:F:217:ALA:HA	2.41	0.51
1:I:67:ARG:HH12	1:I:198:GLU:CD	2.18	0.51
1:A:56:PHE:CG	1:A:66:ILE:HD12	2.46	0.51
1:F:124:PHE:CG	1:F:162:ARG:HG3	2.47	0.51
1:I:82:MET:HE1	1:I:144:VAL:HG21	1.93	0.51
1:J:85:TRP:H	1:J:85:TRP:CD1	2.29	0.50
1:H:22:ASP:O	1:H:25:GLU:HB2	2.12	0.50
1:D:210:ARG:HD2	1:E:186:PHE:CE2	2.46	0.50
1:G:38:LYS:HG2	1:G:110:GLU:HG2	1.93	0.50
1:C:72:LEU:HD23	1:C:230:GLY:HA3	1.93	0.50
1:F:235:ILE:O	1:F:239:VAL:HG23	2.12	0.50
1:G:54:GLU:O	1:G:58:GLN:HG3	2.11	0.50
1:I:132:PHE:HD1	1:I:181:ASN:HD22	1.59	0.50
1:I:133:LEU:C	1:I:135:ASP:H	2.19	0.50
1:B:192:GLU:OE2	1:E:213:ARG:NH1	2.42	0.50
1:G:72:LEU:HD11	1:G:82:MET:HB2	1.94	0.50
1:I:85:TRP:CD1	1:I:85:TRP:N	2.78	0.50
1:J:40:THR:HB	1:J:243:ALA:C	2.37	0.50
1:J:71:ASP:HB2	1:J:233:LYS:HD2	1.94	0.50
1:A:182:THR:HG22	1:A:195:LEU:HG	1.94	0.49
1:A:227:PHE:CE2	1:C:187:SER:HA	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:LYS:HE3	1:D:107:ARG:O	2.11	0.49
1:H:48:TYR:CE1	1:H:104:LYS:HB3	2.47	0.49
1:I:181:ASN:HB2	1:I:196:ALA:HB3	1.94	0.49
1:I:76:ARG:NH2	1:J:190:ASP:OD1	2.46	0.49
1:A:35:PHE:HB3	1:A:109:LEU:HB3	1.94	0.49
1:F:35:PHE:HB3	1:F:109:LEU:HB3	1.94	0.49
1:F:85:TRP:N	1:F:85:TRP:CD1	2.81	0.49
1:I:148:VAL:HA	1:I:192:GLU:HG3	1.93	0.49
1:J:85:TRP:CD1	1:J:85:TRP:N	2.81	0.49
1:I:67:ARG:HG2	1:I:67:ARG:HH11	1.78	0.49
1:D:28:ARG:HH21	1:D:65:THR:HG23	1.77	0.49
1:E:119:HIS:O	1:E:120:ARG:HD2	2.13	0.49
1:F:168:HIS:HE1	2:F:301:VOV:N02	2.09	0.49
1:C:72:LEU:HD11	1:C:82:MET:HB2	1.95	0.48
1:F:45:ARG:NH1	1:F:239:VAL:O	2.44	0.48
1:H:35:PHE:HB3	1:H:109:LEU:HB3	1.95	0.48
1:I:117:ALA:HB1	1:I:183:VAL:HG23	1.94	0.48
1:G:103:THR:O	1:G:107:ARG:HG3	2.13	0.48
1:G:164:MET:HG2	1:G:216:GLU:HB2	1.95	0.48
1:H:160:ASP:OD1	1:H:163:ARG:NH2	2.46	0.48
1:I:76:ARG:HH22	1:J:190:ASP:CG	2.21	0.48
1:H:88:GLU:H	1:H:92:GLN:NE2	2.10	0.48
1:F:115:ASN:HB3	1:F:194:ILE:CD1	2.44	0.48
1:H:23:LEU:C	1:H:25:GLU:H	2.22	0.48
1:F:235:ILE:H	1:F:235:ILE:HD12	1.79	0.48
1:H:41:LEU:H	1:H:242:LEU:CD2	2.26	0.48
1:A:138:PRO:HB2	1:A:232:ARG:HD2	1.95	0.48
1:F:235:ILE:HD12	1:F:235:ILE:N	2.29	0.48
1:J:52:VAL:HG11	1:J:235:ILE:HD13	1.96	0.48
1:B:67:ARG:HG3	1:B:138:PRO:HG3	1.95	0.48
1:F:40:THR:HG21	1:H:107:ARG:NH1	2.29	0.48
1:A:187:SER:HB3	1:B:209:MET:HG3	1.96	0.47
1:G:168:HIS:HE1	2:G:301:VOV:N02	2.11	0.47
1:H:177:ASP:OD1	1:H:177:ASP:N	2.40	0.47
1:J:52:VAL:HG11	1:J:235:ILE:CD1	2.44	0.47
1:C:24:ASN:ND2	1:C:126:ARG:O	2.47	0.47
1:D:62:LYS:H	1:D:62:LYS:HD2	1.78	0.47
1:H:172:ALA:HB1	2:H:301:VOV:C45	2.45	0.47
1:A:55:LEU:O	1:A:59:LEU:HG	2.14	0.47
1:G:49:ALA:HB1	1:G:236:GLY:HA2	1.96	0.47
1:H:140:ASN:HB2	1:H:200:ASP:HA	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:141:TYR:HE1	1:H:231:ARG:HG2	1.80	0.47
1:B:54:GLU:O	1:B:58:GLN:HG3	2.15	0.47
1:F:149:ARG:HD2	1:F:153:TRP:CD2	2.50	0.47
1:A:49:ALA:CB	1:A:236:GLY:HA2	2.44	0.47
1:B:81:LEU:HD23	1:B:82:MET:N	2.30	0.47
1:A:89:THR:HG23	1:A:92:GLN:H	1.80	0.47
1:E:171:MET:HB3	1:E:171:MET:HE2	1.65	0.47
1:I:66:ILE:HG12	1:I:85:TRP:HB3	1.95	0.47
1:C:36:LYS:HB3	1:C:112:VAL:HG21	1.97	0.46
1:A:59:LEU:HB3	1:A:64:VAL:HB	1.98	0.46
1:A:194:ILE:O	1:A:195:LEU:HD12	2.16	0.46
1:B:56:PHE:CD1	1:B:66:ILE:HD13	2.50	0.46
1:C:30:THR:CG2	1:C:132:PHE:CZ	2.98	0.46
1:C:33:SER:HA	1:C:114:SER:HA	1.97	0.46
1:H:85:TRP:N	1:H:85:TRP:CD1	2.82	0.46
1:H:170:LYS:HA	1:H:173:ARG:HD3	1.97	0.46
1:I:141:TYR:CE1	1:I:231:ARG:HD2	2.51	0.46
1:A:178:VAL:HG22	1:A:199:ALA:HB2	1.97	0.46
1:G:101:ARG:NH2	1:J:39:ASP:O	2.49	0.46
1:H:72:LEU:HD11	1:H:82:MET:HB2	1.97	0.46
1:H:150:SER:HA	1:H:222:ARG:HG3	1.97	0.46
1:J:81:LEU:HD23	1:J:82:MET:N	2.30	0.46
1:H:212:LEU:HD23	1:H:212:LEU:HA	1.70	0.46
1:C:24:ASN:ND2	1:C:126:ARG:HB3	2.32	0.45
1:E:218:ARG:NH1	2:E:301:VOV:O15	2.35	0.45
1:F:72:LEU:HD11	1:F:82:MET:HB2	1.97	0.45
1:I:28:ARG:HD3	1:I:87:ALA:O	2.16	0.45
1:C:35:PHE:HB3	1:C:109:LEU:HB3	1.98	0.45
1:A:227:PHE:CD2	1:C:187:SER:HA	2.51	0.45
1:C:82:MET:HE1	1:C:144:VAL:HB	1.98	0.45
1:H:45:ARG:NH1	1:I:102:ARG:HH21	2.12	0.45
1:I:106:GLY:HA2	1:I:109:LEU:HD12	1.97	0.45
1:A:142:ILE:HA	1:A:197:PHE:O	2.16	0.45
1:A:168:HIS:CE1	2:A:301:VOV:N02	2.84	0.45
1:C:212:LEU:HD23	1:C:212:LEU:HA	1.78	0.45
1:H:40:THR:HB	1:H:242:LEU:HD21	1.99	0.45
1:I:216:GLU:OE2	1:I:219:ARG:HD2	2.16	0.45
1:A:85:TRP:CD1	1:A:85:TRP:H	2.35	0.45
1:B:97:TYR:CE1	1:B:101:ARG:HD2	2.51	0.45
1:C:164:MET:O	1:C:168:HIS:HB3	2.16	0.45
1:A:149:ARG:O	1:A:222:ARG:HD3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:85:TRP:CD1	1:F:85:TRP:H	2.35	0.45
1:H:27:ILE:HG13	1:H:27:ILE:O	2.15	0.45
1:A:130:PRO:HB2	1:A:132:PHE:HD1	1.82	0.45
1:F:142:ILE:HA	1:F:197:PHE:O	2.17	0.45
1:F:164:MET:HE2	1:F:217:ALA:HA	1.99	0.45
1:F:182:THR:HB	1:F:195:LEU:HD22	1.99	0.44
1:C:149:ARG:HD2	1:C:153:TRP:CD2	2.51	0.44
1:F:212:LEU:HA	1:F:212:LEU:HD23	1.70	0.44
1:A:203:HIS:NE2	1:A:204:ARG:HD2	2.32	0.44
1:B:49:ALA:HB1	1:B:236:GLY:HA2	2.00	0.44
1:G:23:LEU:HA	1:G:26:VAL:HG23	2.00	0.44
1:A:29:TYR:CE1	1:A:118:LEU:HD13	2.52	0.44
1:H:202:LEU:HD23	1:I:29:TYR:CE2	2.52	0.44
1:F:75:LEU:HD23	1:F:75:LEU:HA	1.67	0.44
1:H:149:ARG:HG3	1:H:153:TRP:CD1	2.53	0.44
1:G:132:PHE:H	1:G:181:ASN:ND2	2.15	0.44
1:I:82:MET:HE1	1:I:144:VAL:CG2	2.48	0.44
1:B:204:ARG:HG3	1:B:204:ARG:HH11	1.83	0.44
1:C:70:TYR:HB2	1:C:82:MET:HB3	1.99	0.44
1:E:53:GLN:HG2	1:E:235:ILE:HG21	2.00	0.44
1:G:128:HIS:C	1:G:129:ILE:HD12	2.43	0.44
1:C:149:ARG:HD2	1:C:153:TRP:CG	2.53	0.43
1:J:35:PHE:HB3	1:J:109:LEU:HB3	1.98	0.43
1:H:149:ARG:NH2	1:H:217:ALA:HB1	2.32	0.43
1:J:54:GLU:O	1:J:58:GLN:HG3	2.19	0.43
1:B:177:ASP:OD1	1:B:177:ASP:N	2.50	0.43
1:C:59:LEU:HD21	1:C:96:ALA:HB1	2.00	0.43
1:J:177:ASP:OD1	1:J:204:ARG:NH1	2.51	0.43
1:E:115:ASN:HB3	1:E:194:ILE:HD11	1.99	0.43
1:F:226:PRO:HG2	1:F:228:TYR:CE2	2.53	0.43
1:G:23:LEU:HD23	1:G:26:VAL:HG21	2.00	0.43
1:I:72:LEU:HD23	1:I:230:GLY:HA3	2.01	0.43
1:J:28:ARG:HD2	1:J:28:ARG:HA	1.86	0.43
1:C:243:ALA:H	1:D:98:ASN:HD22	1.67	0.43
1:I:28:ARG:HG3	1:I:132:PHE:HE2	1.83	0.43
1:F:177:ASP:OD1	1:F:204:ARG:NH1	2.52	0.43
1:A:40:THR:OG1	1:A:243:ALA:O	2.32	0.42
1:B:143:SER:HB2	1:B:229:THR:OG1	2.19	0.42
1:C:210:ARG:HD3	1:D:186:PHE:CZ	2.54	0.42
1:J:168:HIS:HE1	2:J:301:VOV:N02	2.12	0.42
1:A:243:ALA:C	1:C:102:ARG:HE	2.27	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:PHE:CG	1:B:66:ILE:HD13	2.54	0.42
1:E:130:PRO:HD2	1:E:133:LEU:HD12	2.01	0.42
1:J:209:MET:HE1	2:J:301:VOV:C13	2.49	0.42
1:I:182:THR:HG22	1:I:195:LEU:HG	2.01	0.42
1:A:174:GLY:C	1:A:176:PRO:HD3	2.44	0.42
1:A:129:ILE:HG23	1:A:133:LEU:HD12	2.00	0.42
1:B:210:ARG:HD2	1:B:210:ARG:O	2.19	0.42
1:F:149:ARG:HD2	1:F:153:TRP:CD1	2.53	0.42
1:A:176:PRO:O	1:A:179:ARG:NH1	2.52	0.42
1:F:52:VAL:HG21	1:F:105:LEU:HD23	2.02	0.42
1:G:149:ARG:HD3	1:G:153:TRP:CG	2.54	0.42
1:C:31:LEU:HD12	1:C:115:ASN:O	2.20	0.42
1:G:139:ARG:HB2	1:G:198:GLU:HB3	2.02	0.42
1:J:28:ARG:NH2	1:J:65:THR:HG23	2.35	0.42
1:C:149:ARG:HH21	2:C:301:VOV:C22	2.33	0.42
1:C:39:ASP:HB3	1:C:40:THR:H	1.61	0.42
1:D:85:TRP:CD1	1:D:85:TRP:N	2.88	0.42
1:F:65:THR:OG1	1:F:86:HIS:NE2	2.53	0.42
1:G:40:THR:HB	1:G:243:ALA:C	2.44	0.42
1:G:119:HIS:O	1:G:120:ARG:HD2	2.19	0.42
1:H:46:ALA:C	1:H:48:TYR:H	2.28	0.42
1:J:41:LEU:HD23	1:J:41:LEU:HA	1.86	0.42
1:E:166:ALA:O	1:E:170:LYS:HG2	2.20	0.42
1:I:35:PHE:HB3	1:I:109:LEU:HB3	2.02	0.42
1:I:36:LYS:HD3	1:I:112:VAL:HG22	2.01	0.42
1:J:146:PRO:HB2	1:J:191:TYR:CD1	2.54	0.42
1:A:89:THR:HG22	1:A:92:GLN:OE1	2.20	0.41
1:A:143:SER:HB2	1:A:229:THR:OG1	2.19	0.41
1:C:59:LEU:HD12	1:C:59:LEU:HA	1.88	0.41
1:C:77:ALA:HB1	1:D:111:PRO:HB2	2.02	0.41
1:C:130:PRO:HB2	1:C:132:PHE:CD1	2.55	0.41
1:E:85:TRP:CD1	1:E:85:TRP:N	2.86	0.41
1:I:233:LYS:HD3	1:I:237:GLU:HG2	2.00	0.41
1:C:31:LEU:O	1:C:85:TRP:HD1	2.03	0.41
1:C:97:TYR:HE1	1:C:101:ARG:HD2	1.84	0.41
1:C:150:SER:HA	1:C:222:ARG:HG3	2.02	0.41
1:D:235:ILE:O	1:D:239:VAL:HG23	2.20	0.41
1:G:85:TRP:CD1	1:G:85:TRP:N	2.89	0.41
1:J:45:ARG:NH1	1:J:239:VAL:O	2.54	0.41
1:A:149:ARG:HD2	1:A:153:TRP:CE2	2.55	0.41
1:D:29:TYR:CD1	1:D:118:LEU:HB2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:PHE:CE2	1:D:192:GLU:HB3	2.55	0.41
1:B:35:PHE:HB3	1:B:109:LEU:HB3	2.02	0.41
1:F:99:LEU:HD23	1:F:99:LEU:HA	1.75	0.41
1:G:133:LEU:HD23	1:G:133:LEU:HA	1.74	0.41
1:J:177:ASP:CG	1:J:204:ARG:HH11	2.29	0.41
1:H:147:PHE:HB2	1:H:195:LEU:HD13	2.02	0.41
1:B:23:LEU:HD23	1:B:23:LEU:HA	1.90	0.41
1:F:162:ARG:CZ	1:F:162:ARG:HB3	2.50	0.41
1:I:85:TRP:H	1:I:85:TRP:HD1	1.68	0.41
1:G:149:ARG:HD3	1:G:153:TRP:NE1	2.35	0.41
1:J:146:PRO:O	1:J:224:GLU:HA	2.21	0.41
1:A:235:ILE:H	1:A:235:ILE:CD1	2.25	0.41
1:B:159:GLU:OE1	1:B:162:ARG:HD2	2.20	0.41
1:C:35:PHE:HB2	1:C:109:LEU:HD13	2.02	0.41
1:C:48:TYR:CE2	1:C:104:LYS:HG2	2.56	0.41
1:C:49:ALA:HB1	1:C:236:GLY:HA2	2.02	0.41
1:G:153:TRP:CZ2	1:G:161:ARG:HG3	2.56	0.41
1:G:182:THR:HB	1:G:195:LEU:HD22	2.03	0.41
1:H:41:LEU:HB2	1:H:242:LEU:HD23	2.02	0.41
1:J:45:ARG:O	1:J:46:ALA:C	2.63	0.41
1:E:97:TYR:CE1	1:E:101:ARG:HD2	2.56	0.41
1:H:136:GLU:CD	1:H:179:ARG:HH11	2.29	0.41
1:G:177:ASP:OD1	1:G:177:ASP:N	2.50	0.40
1:G:41:LEU:HB2	1:G:45:ARG:NH2	2.37	0.40
1:I:138:PRO:HB2	1:I:232:ARG:HE	1.86	0.40
1:A:141:TYR:O	1:A:198:GLU:HA	2.21	0.40
1:D:66:ILE:HD12	1:D:66:ILE:N	2.36	0.40
1:I:130:PRO:CG	1:I:183:VAL:HG12	2.51	0.40
1:A:149:ARG:HD2	1:A:153:TRP:CD1	2.57	0.40
1:C:149:ARG:HG3	1:C:153:TRP:CD1	2.57	0.40
1:G:55:LEU:O	1:G:59:LEU:HG	2.21	0.40
1:G:102:ARG:NH1	1:J:45:ARG:NH2	2.68	0.40
1:H:70:TYR:CE2	1:H:142:ILE:HB	2.57	0.40
1:J:123:GLU:OE2	1:J:124:PHE:CZ	2.75	0.40
1:F:168:HIS:HE1	2:F:301:VOV:C07	2.35	0.40
1:H:22:ASP:OD1	1:H:22:ASP:N	2.55	0.40
1:H:149:ARG:HH22	1:H:217:ALA:HB1	1.87	0.40
1:I:49:ALA:CB	1:I:236:GLY:HA2	2.52	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	219/243 (90%)	202 (92%)	14 (6%)	3 (1%)	9 17
1	B	220/243 (90%)	206 (94%)	13 (6%)	1 (0%)	24 43
1	C	219/243 (90%)	203 (93%)	15 (7%)	1 (0%)	24 43
1	D	220/243 (90%)	206 (94%)	14 (6%)	0	100 100
1	E	216/243 (89%)	203 (94%)	12 (6%)	1 (0%)	24 43
1	F	219/243 (90%)	203 (93%)	13 (6%)	3 (1%)	9 17
1	G	220/243 (90%)	206 (94%)	14 (6%)	0	100 100
1	H	219/243 (90%)	201 (92%)	17 (8%)	1 (0%)	24 43
1	I	219/243 (90%)	200 (91%)	15 (7%)	4 (2%)	6 12
1	J	220/243 (90%)	206 (94%)	12 (6%)	2 (1%)	14 27
All	All	2191/2430 (90%)	2036 (93%)	139 (6%)	16 (1%)	18 34

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	135	ASP
1	J	24	ASN
1	A	131	ALA
1	A	135	ASP
1	F	46	ALA
1	I	63	ASP
1	I	103	THR
1	I	135	ASP
1	J	46	ALA
1	H	46	ALA
1	A	62	LYS
1	I	134	ALA
1	B	46	ALA
1	C	24	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	27	ILE
1	F	64	VAL

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	187/204 (92%)	184 (98%)	3 (2%)	55 79
1	B	188/204 (92%)	180 (96%)	8 (4%)	26 51
1	C	187/204 (92%)	185 (99%)	2 (1%)	65 84
1	D	188/204 (92%)	179 (95%)	9 (5%)	23 46
1	E	184/204 (90%)	181 (98%)	3 (2%)	55 79
1	F	187/204 (92%)	178 (95%)	9 (5%)	23 46
1	G	188/204 (92%)	184 (98%)	4 (2%)	47 74
1	H	188/204 (92%)	181 (96%)	7 (4%)	30 57
1	I	187/204 (92%)	180 (96%)	7 (4%)	30 57
1	J	188/204 (92%)	181 (96%)	7 (4%)	30 57
All	All	1872/2040 (92%)	1813 (97%)	59 (3%)	34 62

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	TRP
1	A	168	HIS
1	A	231	ARG
1	B	38	LYS
1	B	45	ARG
1	B	85	TRP
1	B	168	HIS
1	B	182	THR
1	B	187	SER
1	B	205	ILE
1	B	212	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	85	TRP
1	C	168	HIS
1	D	39	ASP
1	D	65	THR
1	D	75	LEU
1	D	85	TRP
1	D	114	SER
1	D	133	LEU
1	D	168	HIS
1	D	205	ILE
1	D	225	ILE
1	E	85	TRP
1	E	168	HIS
1	E	187	SER
1	F	40	THR
1	F	85	TRP
1	F	137	THR
1	F	168	HIS
1	F	183	VAL
1	F	185	SER
1	F	187	SER
1	F	204	ARG
1	F	234	ASP
1	G	85	TRP
1	G	149	ARG
1	G	168	HIS
1	G	183	VAL
1	H	26	VAL
1	H	38	LYS
1	H	58	GLN
1	H	85	TRP
1	H	181	ASN
1	H	183	VAL
1	H	229	THR
1	I	30	THR
1	I	55	LEU
1	I	81	LEU
1	I	85	TRP
1	I	137	THR
1	I	168	HIS
1	I	187	SER
1	J	30	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	65	THR
1	J	85	TRP
1	J	168	HIS
1	J	187	SER
1	J	215	SER
1	J	238	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	119	HIS
1	A	128	HIS
1	A	168	HIS
1	A	181	ASN
1	A	220	HIS
1	B	115	ASN
1	C	119	HIS
1	C	181	ASN
1	D	168	HIS
1	D	211	HIS
1	E	58	GLN
1	E	92	GLN
1	E	203	HIS
1	F	92	GLN
1	G	24	ASN
1	G	58	GLN
1	G	92	GLN
1	G	128	HIS
1	G	168	HIS
1	G	181	ASN
1	G	203	HIS
1	H	24	ASN
1	H	92	GLN
1	H	119	HIS
1	H	203	HIS
1	I	168	HIS
1	J	211	HIS

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

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	VOV	F	301	1	53,53,53	1.04	6 (11%)	72,86,86	1.31	8 (11%)
2	VOV	J	301	1	53,53,53	1.05	5 (9%)	72,86,86	1.20	7 (9%)
2	VOV	D	301	1	53,53,53	1.00	5 (9%)	72,86,86	1.34	11 (15%)
2	VOV	E	301	1	53,53,53	1.07	4 (7%)	72,86,86	1.29	9 (12%)
2	VOV	H	301	1	53,53,53	1.05	4 (7%)	72,86,86	1.09	7 (9%)
2	VOV	G	301	1	53,53,53	1.10	5 (9%)	72,86,86	1.36	11 (15%)
2	VOV	A	301	1	53,53,53	1.11	6 (11%)	72,86,86	1.35	10 (13%)
2	VOV	I	301	1	53,53,53	0.99	5 (9%)	72,86,86	1.29	8 (11%)
2	VOV	B	301	1	53,53,53	1.00	4 (7%)	72,86,86	1.29	11 (15%)
2	VOV	C	301	1	53,53,53	1.18	6 (11%)	72,86,86	1.38	11 (15%)

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	VOV	F	301	1	1/1/4/9	10/17/57/57	-
2	VOV	J	301	1	1/1/4/9	11/17/57/57	-
2	VOV	D	301	1	1/1/4/9	8/17/57/57	-
2	VOV	E	301	1	1/1/4/9	10/17/57/57	-
2	VOV	H	301	1	1/1/4/9	8/17/57/57	-
2	VOV	G	301	1	1/1/4/9	9/17/57/57	-
2	VOV	A	301	1	1/1/4/9	11/17/57/57	-
2	VOV	I	301	1	1/1/4/9	10/17/57/57	-
2	VOV	B	301	1	1/1/4/9	11/17/57/57	-
2	VOV	C	301	1	1/1/4/9	9/17/57/57	-

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	VOV	FE-N03	3.98	2.07	1.94
2	J	301	VOV	C28-C29	3.70	1.47	1.39
2	G	301	VOV	C28-C29	3.62	1.47	1.39
2	C	301	VOV	C28-C29	3.48	1.47	1.39
2	A	301	VOV	C28-C29	3.46	1.47	1.39
2	C	301	VOV	FE-N03	3.38	2.05	1.94
2	H	301	VOV	FE-N03	3.24	2.04	1.94
2	B	301	VOV	FE-N03	3.18	2.04	1.94
2	E	301	VOV	C28-C29	3.02	1.46	1.39
2	D	301	VOV	FE-N03	3.01	2.04	1.94
2	J	301	VOV	FE-N03	2.96	2.04	1.94
2	A	301	VOV	FE-N03	2.91	2.03	1.94
2	I	301	VOV	C28-C29	2.89	1.45	1.39
2	C	301	VOV	FE-N04	2.75	2.04	1.95
2	H	301	VOV	FE-N05	2.68	2.03	1.94
2	G	301	VOV	FE-N03	2.64	2.03	1.94
2	F	301	VOV	FE-N03	2.61	2.02	1.94
2	F	301	VOV	FE-N04	2.59	2.03	1.95
2	G	301	VOV	FE-N05	2.58	2.02	1.94
2	G	301	VOV	FE-N04	2.54	2.03	1.95
2	I	301	VOV	FE-N03	2.54	2.02	1.94
2	D	301	VOV	FE-N02	2.50	2.03	1.95
2	A	301	VOV	FE-N02	2.48	2.03	1.95
2	D	301	VOV	C28-C29	2.45	1.44	1.39
2	H	301	VOV	FE-N04	2.43	2.03	1.95
2	B	301	VOV	FE-N05	2.42	2.02	1.94
2	J	301	VOV	FE-N04	2.42	2.03	1.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	VOV	FE-N05	2.42	2.02	1.94
2	G	301	VOV	C06-C07	2.42	1.43	1.38
2	I	301	VOV	FE-N04	2.41	2.03	1.95
2	F	301	VOV	C28-C29	2.41	1.44	1.39
2	A	301	VOV	FE-N05	2.40	2.02	1.94
2	C	301	VOV	FE-N05	2.35	2.02	1.94
2	F	301	VOV	FE-N02	2.34	2.02	1.95
2	D	301	VOV	FE-N04	2.33	2.02	1.95
2	E	301	VOV	FE-N04	2.33	2.02	1.95
2	B	301	VOV	C28-C29	2.31	1.44	1.39
2	F	301	VOV	C06-C07	2.30	1.42	1.38
2	C	301	VOV	FE-N02	2.29	2.02	1.95
2	J	301	VOV	FE-N02	2.23	2.02	1.95
2	A	301	VOV	C06-C07	2.19	1.42	1.38
2	A	301	VOV	FE-N04	2.19	2.02	1.95
2	J	301	VOV	FE-N05	2.17	2.01	1.94
2	I	301	VOV	C06-C07	2.16	1.42	1.38
2	C	301	VOV	C23-C20	2.13	1.56	1.51
2	D	301	VOV	FE-N05	2.12	2.01	1.94
2	H	301	VOV	C06-C07	2.07	1.42	1.38
2	B	301	VOV	FE-N04	2.07	2.02	1.95
2	E	301	VOV	C06-C07	2.06	1.42	1.38
2	I	301	VOV	FE-N05	2.04	2.01	1.94

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	301	VOV	C06-C07-N02	-5.57	118.39	124.45
2	I	301	VOV	C06-C07-N02	-5.51	118.45	124.45
2	J	301	VOV	C06-C07-N02	-4.96	119.05	124.45
2	A	301	VOV	C06-C07-N02	-4.76	119.27	124.45
2	G	301	VOV	C06-C07-N02	-4.76	119.27	124.45
2	B	301	VOV	C06-C07-N02	-4.46	119.59	124.45
2	E	301	VOV	C06-C07-N02	-4.37	119.69	124.45
2	F	301	VOV	C06-C07-N02	-4.34	119.73	124.45
2	C	301	VOV	C06-C07-N02	-4.33	119.74	124.45
2	B	301	VOV	C42-C43-N05	3.88	112.25	109.47
2	F	301	VOV	C17-C10-N02	-3.73	120.39	124.45
2	E	301	VOV	C42-C43-N05	3.64	112.08	109.47
2	H	301	VOV	C06-C07-N02	-3.58	120.56	124.45
2	C	301	VOV	C20-C21-N03	3.57	114.08	110.17
2	C	301	VOV	C28-C21-N03	-3.50	120.03	124.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	VOV	C17-C18-C19	3.42	130.43	125.03
2	E	301	VOV	C39-C40-N05	-3.25	120.35	124.37
2	B	301	VOV	C23-C20-C21	3.24	130.34	124.70
2	I	301	VOV	C17-C10-N02	-3.23	120.93	124.45
2	G	301	VOV	C42-C43-N05	3.14	111.72	109.47
2	F	301	VOV	C17-C18-C19	3.10	129.93	125.03
2	G	301	VOV	C17-C18-C19	3.10	129.92	125.03
2	C	301	VOV	C21-C20-C19	-3.09	102.39	106.89
2	A	301	VOV	C23-C20-C21	3.05	130.01	124.70
2	I	301	VOV	C06-C07-C08	2.98	131.69	125.49
2	A	301	VOV	C17-C10-N02	-2.86	121.34	124.45
2	E	301	VOV	C17-C18-C19	2.81	129.47	125.03
2	G	301	VOV	C39-C40-N05	-2.78	120.93	124.37
2	G	301	VOV	C17-C18-N03	-2.74	121.47	124.42
2	H	301	VOV	C17-C18-N03	-2.74	121.48	124.42
2	B	301	VOV	C20-C21-N03	2.74	113.17	110.17
2	G	301	VOV	C06-C07-C08	2.74	131.18	125.49
2	F	301	VOV	C18-C19-C20	2.71	109.83	106.98
2	A	301	VOV	C17-C18-N03	-2.71	121.51	124.42
2	H	301	VOV	C17-C18-C19	2.70	129.29	125.03
2	D	301	VOV	C20-C21-N03	2.70	113.13	110.17
2	D	301	VOV	C06-C07-C08	2.69	131.09	125.49
2	I	301	VOV	C23-C20-C21	2.68	129.37	124.70
2	A	301	VOV	C06-C07-C08	2.66	131.02	125.49
2	H	301	VOV	C42-C43-N05	2.66	111.38	109.47
2	B	301	VOV	C28-C21-N03	-2.61	121.14	124.37
2	H	301	VOV	C20-C21-N03	2.60	113.03	110.17
2	D	301	VOV	C42-C43-N05	2.58	111.32	109.47
2	B	301	VOV	C06-C43-N05	-2.53	121.70	124.42
2	B	301	VOV	C17-C18-N03	-2.51	121.72	124.42
2	C	301	VOV	C17-C18-N03	-2.51	121.73	124.42
2	J	301	VOV	C06-C07-C08	2.47	130.62	125.49
2	C	301	VOV	C23-C20-C21	2.45	128.97	124.70
2	J	301	VOV	C23-C20-C21	2.45	128.97	124.70
2	G	301	VOV	C06-C43-N05	-2.44	121.80	124.42
2	F	301	VOV	C06-C07-C08	2.43	130.54	125.49
2	E	301	VOV	C06-C07-C08	2.43	130.54	125.49
2	A	301	VOV	C18-C19-C20	2.40	109.51	106.98
2	B	301	VOV	C06-C07-C08	2.39	130.45	125.49
2	E	301	VOV	C18-C19-C20	2.34	109.44	106.98
2	F	301	VOV	C42-C43-N05	2.34	111.15	109.47
2	D	301	VOV	C17-C18-N03	-2.33	121.91	124.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	VOV	C07-C06-C43	2.32	130.96	126.02
2	D	301	VOV	C17-C10-N02	-2.32	121.92	124.45
2	J	301	VOV	C42-C43-N05	2.32	111.13	109.47
2	D	301	VOV	C17-C18-C19	2.30	128.66	125.03
2	J	301	VOV	C20-C21-N03	2.29	112.68	110.17
2	D	301	VOV	C39-C40-N05	-2.26	121.57	124.37
2	C	301	VOV	C42-C43-N05	2.26	111.09	109.47
2	C	301	VOV	C24-C23-C20	2.24	118.72	112.53
2	G	301	VOV	C23-C20-C21	2.23	128.57	124.70
2	F	301	VOV	C17-C10-C09	2.22	128.38	124.86
2	G	301	VOV	C28-C29-N04	-2.21	119.85	123.86
2	A	301	VOV	C39-C40-N05	-2.21	121.63	124.37
2	D	301	VOV	C07-C06-C43	2.21	130.72	126.02
2	B	301	VOV	C21-C20-C19	-2.20	103.69	106.89
2	H	301	VOV	C06-C07-C08	2.20	130.06	125.49
2	G	301	VOV	C17-C10-N02	-2.19	122.07	124.45
2	J	301	VOV	C28-C21-N03	-2.19	121.66	124.37
2	I	301	VOV	C17-C18-C19	2.19	128.48	125.03
2	A	301	VOV	C42-C43-N05	2.14	111.01	109.47
2	C	301	VOV	C17-C10-N02	-2.14	122.12	124.45
2	C	301	VOV	C06-C07-C08	2.13	129.92	125.49
2	I	301	VOV	C42-C43-N05	2.13	111.00	109.47
2	E	301	VOV	C06-C43-N05	-2.12	122.14	124.42
2	D	301	VOV	C21-C20-C19	-2.11	103.82	106.89
2	D	301	VOV	C28-C21-N03	-2.10	121.77	124.37
2	I	301	VOV	C39-C40-N05	-2.10	121.77	124.37
2	E	301	VOV	C39-C32-N04	-2.10	120.05	123.86
2	J	301	VOV	C21-C20-C19	-2.07	103.88	106.89
2	B	301	VOV	C17-C18-C19	2.05	128.27	125.03
2	E	301	VOV	C28-C29-N04	-2.05	120.14	123.86
2	I	301	VOV	C18-C19-C20	2.05	109.13	106.98
2	F	301	VOV	C17-C18-N03	-2.04	122.22	124.42
2	H	301	VOV	C21-C20-C19	-2.04	103.93	106.89
2	A	301	VOV	C13-C12-C09	2.03	118.16	112.53
2	C	301	VOV	C18-C19-C20	2.03	109.11	106.98
2	G	301	VOV	C28-C29-C30	2.02	129.73	125.30

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	301	VOV	N02
2	B	301	VOV	N02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
2	C	301	VOV	N02
2	D	301	VOV	N02
2	E	301	VOV	N02
2	F	301	VOV	N02
2	G	301	VOV	N02
2	H	301	VOV	N02
2	I	301	VOV	N02
2	J	301	VOV	N02

All (97) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	VOV	C41-C42-C45-C46
2	A	301	VOV	C43-C42-C45-C46
2	B	301	VOV	C41-C42-C45-C46
2	C	301	VOV	C41-C42-C45-C46
2	D	301	VOV	C41-C42-C45-C46
2	E	301	VOV	C08-C09-C12-C13
2	E	301	VOV	C10-C09-C12-C13
2	E	301	VOV	C41-C42-C45-C46
2	E	301	VOV	C43-C42-C45-C46
2	F	301	VOV	C41-C42-C45-C46
2	G	301	VOV	C41-C42-C45-C46
2	H	301	VOV	C41-C42-C45-C46
2	I	301	VOV	C41-C42-C45-C46
2	I	301	VOV	C43-C42-C45-C46
2	J	301	VOV	C41-C42-C45-C46
2	J	301	VOV	C43-C42-C45-C46
2	H	301	VOV	C08-C09-C12-C13
2	I	301	VOV	C08-C09-C12-C13
2	J	301	VOV	C08-C09-C12-C13
2	H	301	VOV	C10-C09-C12-C13
2	I	301	VOV	C10-C09-C12-C13
2	F	301	VOV	C30-C34-C35-C36
2	I	301	VOV	C30-C34-C35-C36
2	J	301	VOV	C10-C09-C12-C13
2	E	301	VOV	C30-C34-C35-C36
2	J	301	VOV	C30-C34-C35-C36
2	A	301	VOV	C30-C34-C35-C36
2	G	301	VOV	C30-C34-C35-C36
2	C	301	VOV	C10-C09-C12-C13
2	D	301	VOV	C10-C09-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	301	VOV	C43-C42-C45-C46
2	D	301	VOV	C43-C42-C45-C46
2	F	301	VOV	C43-C42-C45-C46
2	H	301	VOV	C43-C42-C45-C46
2	A	301	VOV	C20-C23-C24-C25
2	C	301	VOV	C30-C34-C35-C36
2	H	301	VOV	C30-C34-C35-C36
2	C	301	VOV	C08-C09-C12-C13
2	D	301	VOV	C08-C09-C12-C13
2	B	301	VOV	C20-C23-C24-C25
2	A	301	VOV	C10-C09-C12-C13
2	B	301	VOV	C10-C09-C12-C13
2	F	301	VOV	C10-C09-C12-C13
2	I	301	VOV	C20-C23-C24-C25
2	B	301	VOV	C08-C09-C12-C13
2	F	301	VOV	C20-C23-C24-C25
2	J	301	VOV	C20-C23-C24-C25
2	B	301	VOV	C43-C42-C45-C46
2	G	301	VOV	C43-C42-C45-C46
2	A	301	VOV	C08-C09-C12-C13
2	B	301	VOV	C19-C20-C23-C24
2	F	301	VOV	C08-C09-C12-C13
2	B	301	VOV	C21-C20-C23-C24
2	E	301	VOV	C20-C23-C24-C25
2	F	301	VOV	C34-C35-C36-O38
2	J	301	VOV	C34-C35-C36-O38
2	A	301	VOV	C34-C35-C36-O38
2	D	301	VOV	C30-C34-C35-C36
2	I	301	VOV	C34-C35-C36-O37
2	I	301	VOV	C34-C35-C36-O38
2	E	301	VOV	C12-C13-C14-O15
2	A	301	VOV	C12-C13-C14-O16
2	G	301	VOV	C20-C23-C24-C25
2	G	301	VOV	C34-C35-C36-O38
2	D	301	VOV	C12-C13-C14-O16
2	E	301	VOV	C34-C35-C36-O37
2	B	301	VOV	C34-C35-C36-O38
2	J	301	VOV	C12-C13-C14-O16
2	B	301	VOV	C12-C13-C14-O16
2	B	301	VOV	C34-C35-C36-O37
2	F	301	VOV	C34-C35-C36-O37
2	A	301	VOV	C34-C35-C36-O37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	G	301	VOV	C12-C13-C14-O16
2	G	301	VOV	C34-C35-C36-O37
2	F	301	VOV	C12-C13-C14-O16
2	C	301	VOV	C12-C13-C14-O16
2	D	301	VOV	C34-C35-C36-O38
2	G	301	VOV	C12-C13-C14-O15
2	C	301	VOV	C12-C13-C14-O15
2	J	301	VOV	C12-C13-C14-O15
2	E	301	VOV	C34-C35-C36-O38
2	C	301	VOV	C34-C35-C36-O38
2	F	301	VOV	C12-C13-C14-O15
2	C	301	VOV	C34-C35-C36-O37
2	D	301	VOV	C34-C35-C36-O37
2	J	301	VOV	C34-C35-C36-O37
2	H	301	VOV	C34-C35-C36-O37
2	H	301	VOV	C34-C35-C36-O38
2	A	301	VOV	C19-C20-C23-C24
2	G	301	VOV	C23-C24-C25-O27
2	B	301	VOV	C12-C13-C14-O15
2	E	301	VOV	C12-C13-C14-O16
2	A	301	VOV	C12-C13-C14-O15
2	I	301	VOV	C12-C13-C14-O15
2	I	301	VOV	C12-C13-C14-O16
2	H	301	VOV	C12-C13-C14-O15
2	J	301	VOV	C23-C24-C25-O27

There are no ring outliers.

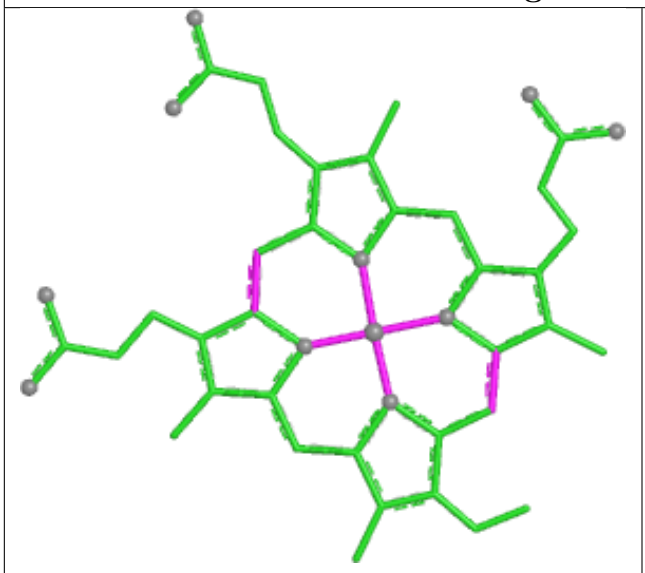
9 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	VOV	2	0
2	J	301	VOV	3	0
2	E	301	VOV	1	0
2	H	301	VOV	2	0
2	G	301	VOV	1	0
2	A	301	VOV	2	0
2	I	301	VOV	1	0
2	B	301	VOV	1	0
2	C	301	VOV	3	0

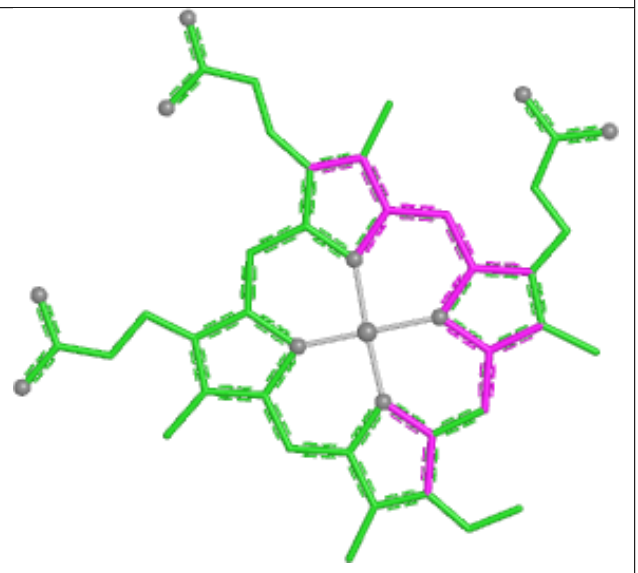
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

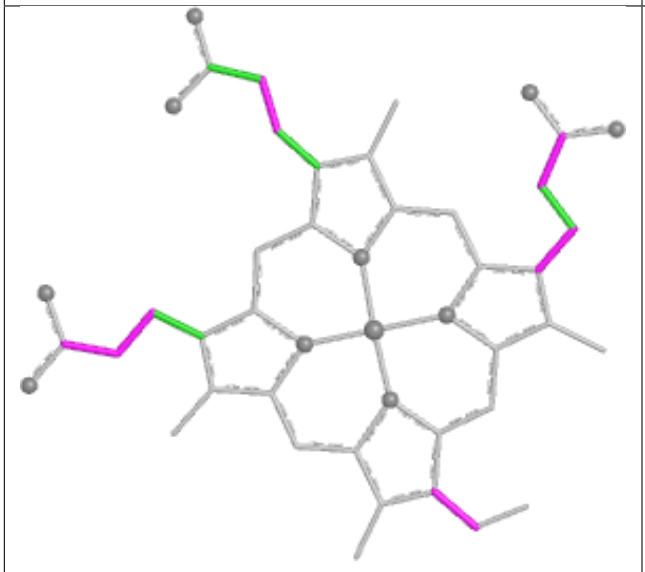
Ligand VOV F 301



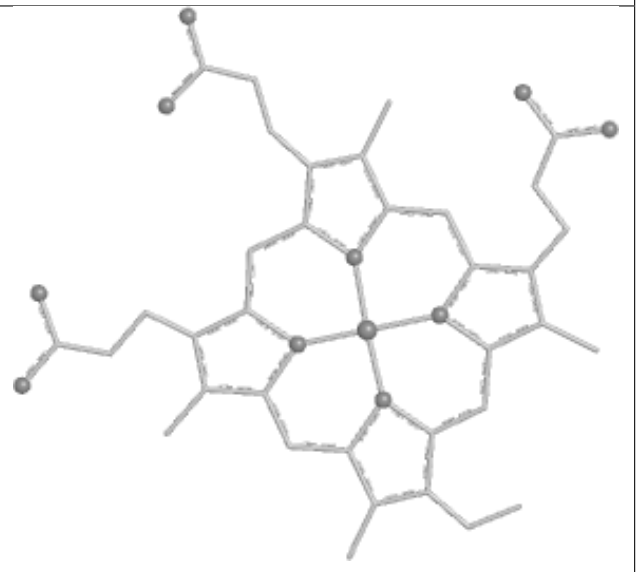
Bond lengths



Bond angles

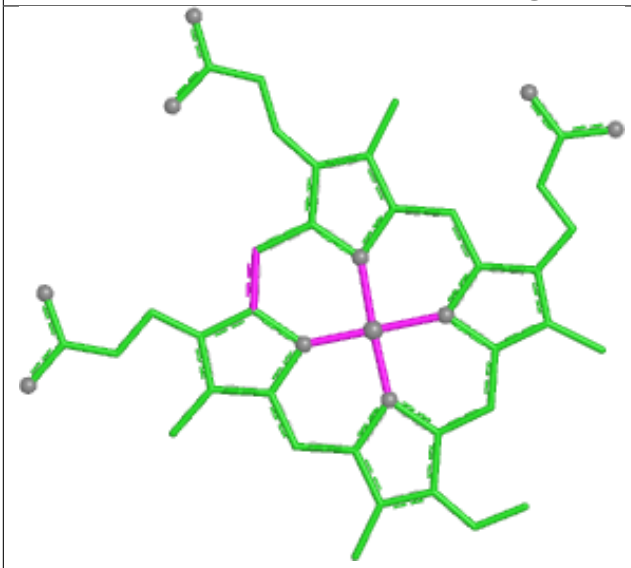


Torsions

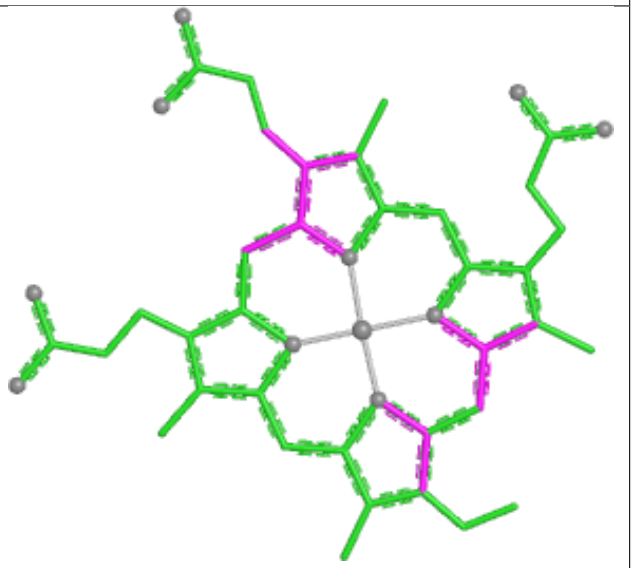


Rings

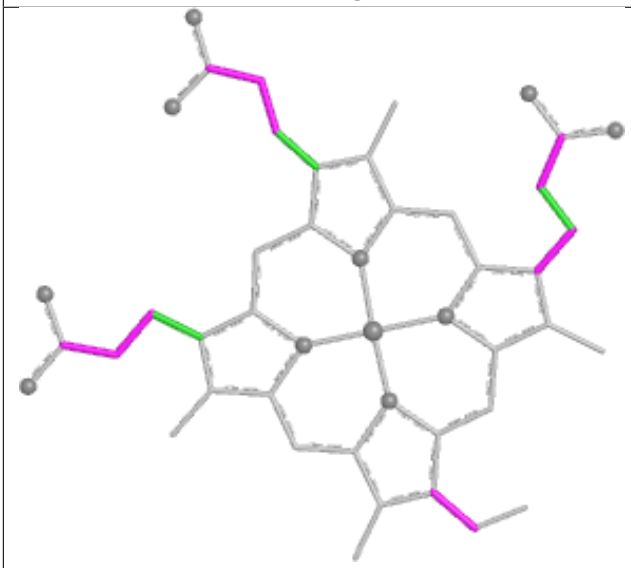
Ligand VOV J 301



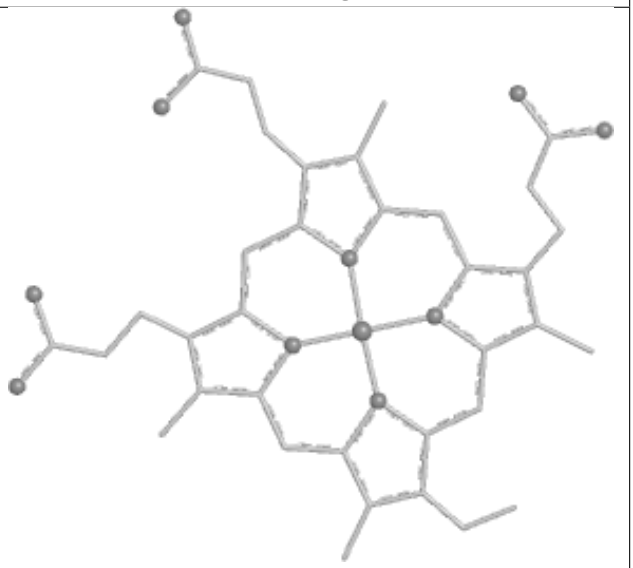
Bond lengths



Bond angles

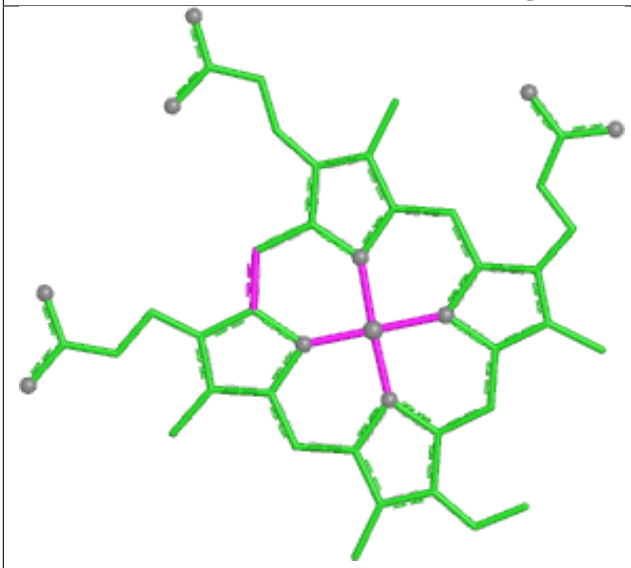


Torsions

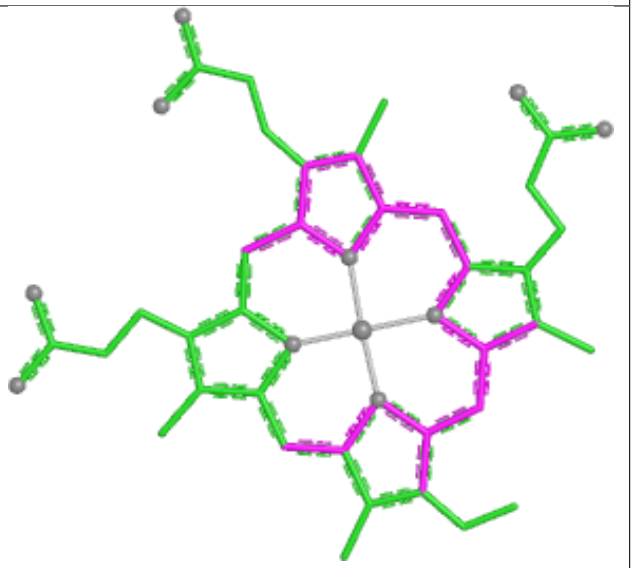


Rings

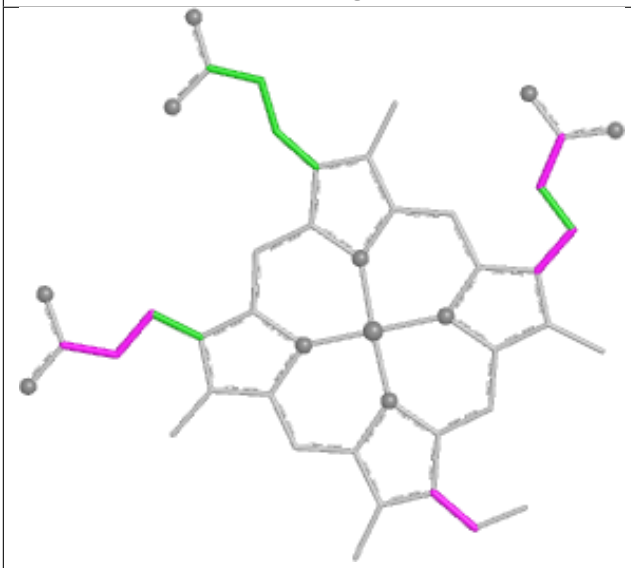
Ligand VOV D 301



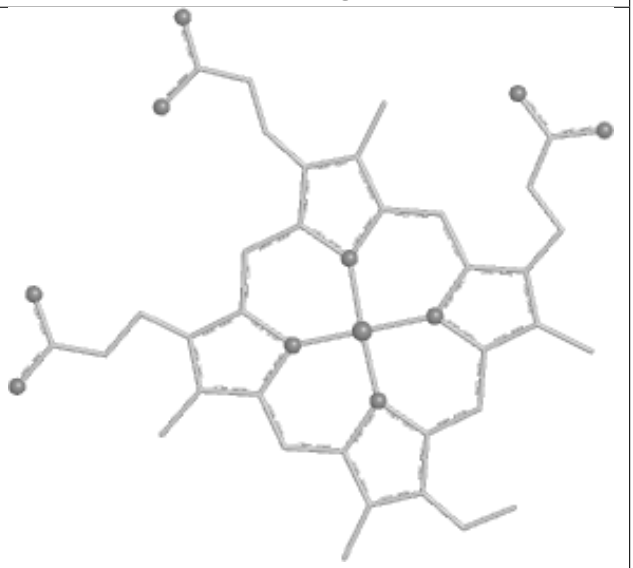
Bond lengths



Bond angles

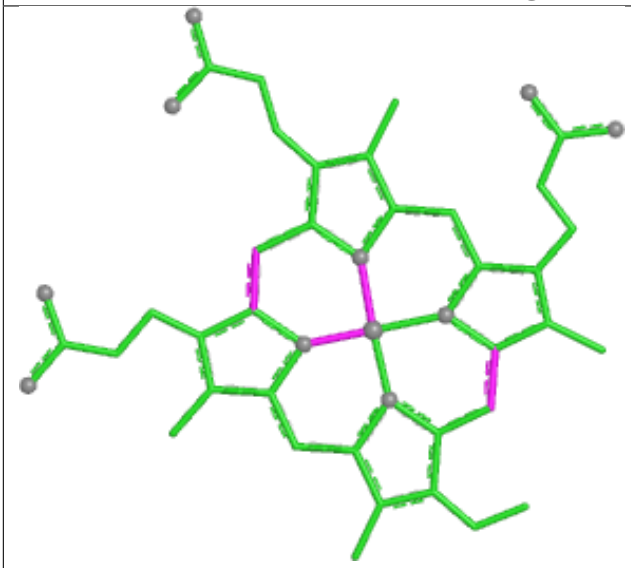


Torsions

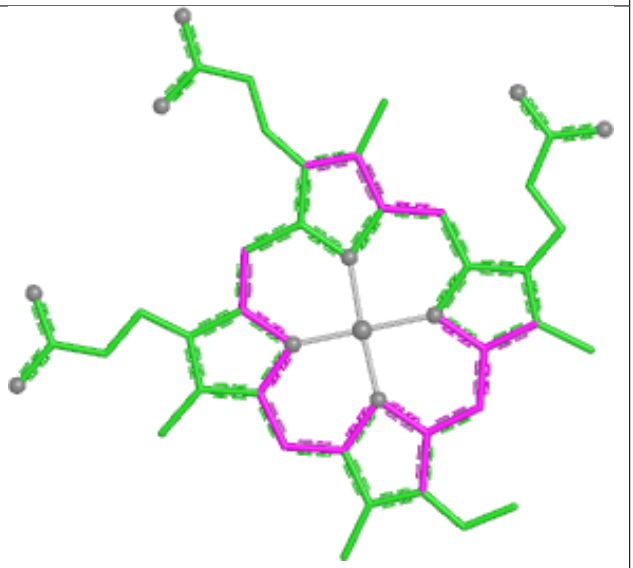


Rings

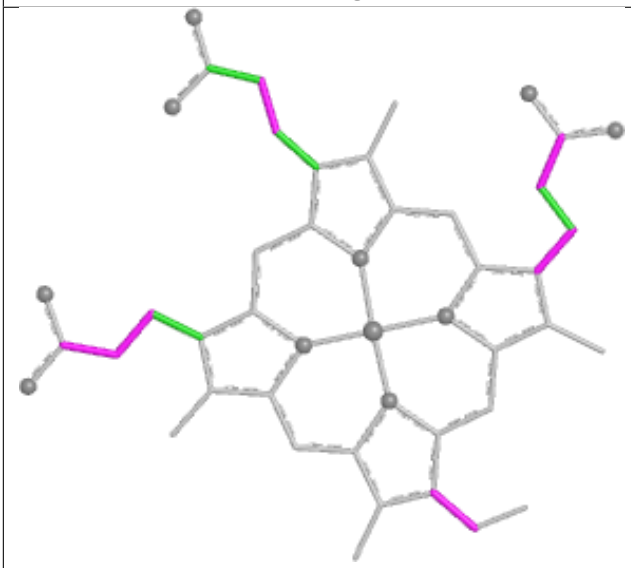
Ligand VOV E 301



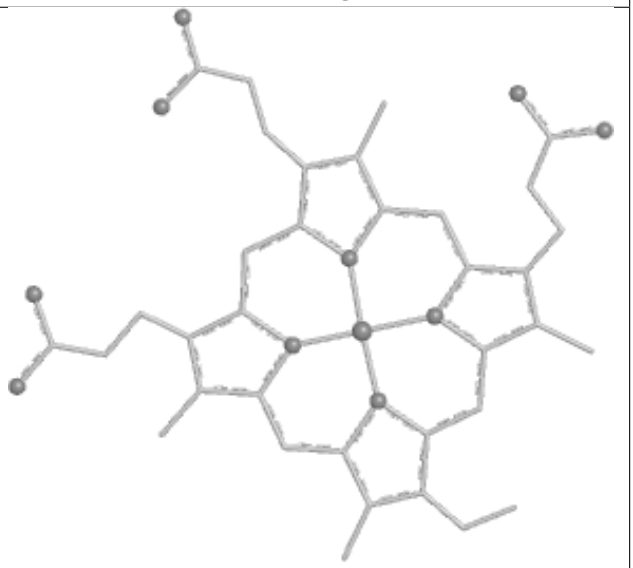
Bond lengths



Bond angles

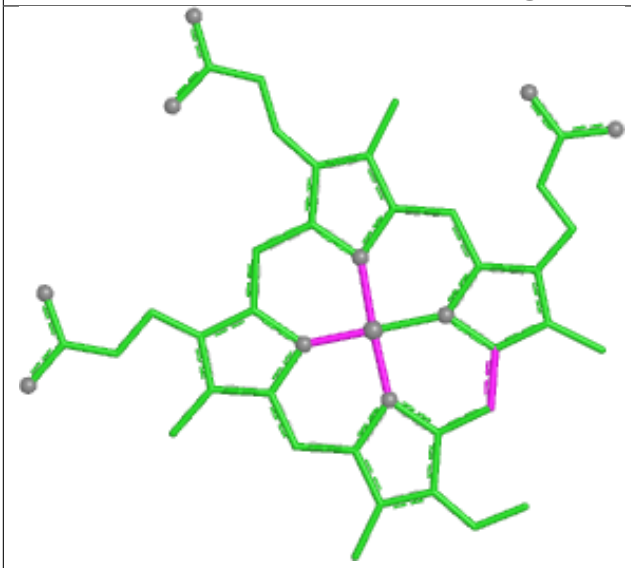


Torsions

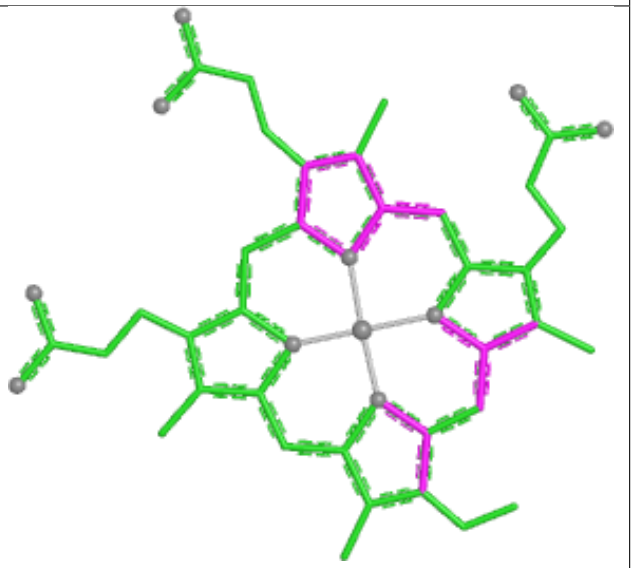


Rings

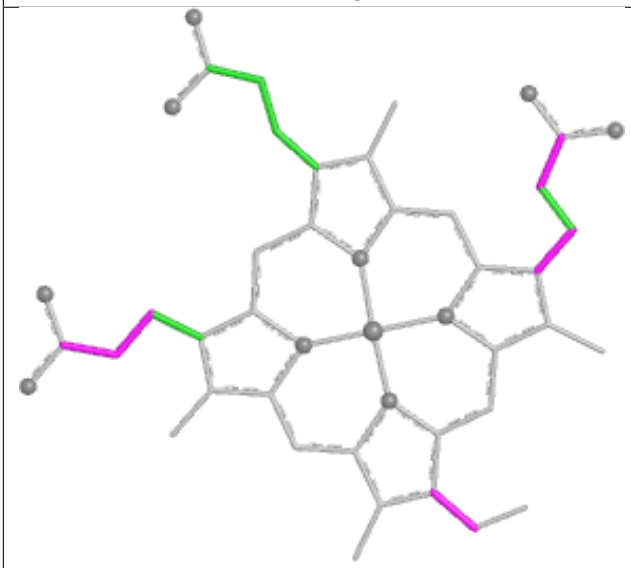
Ligand VOV H 301



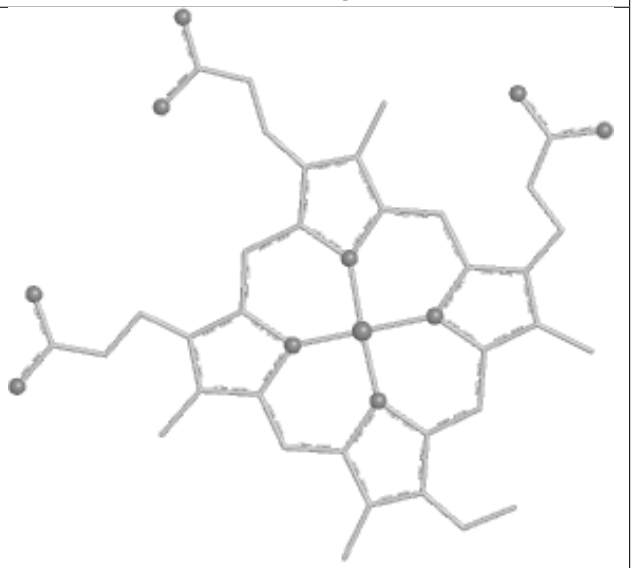
Bond lengths



Bond angles

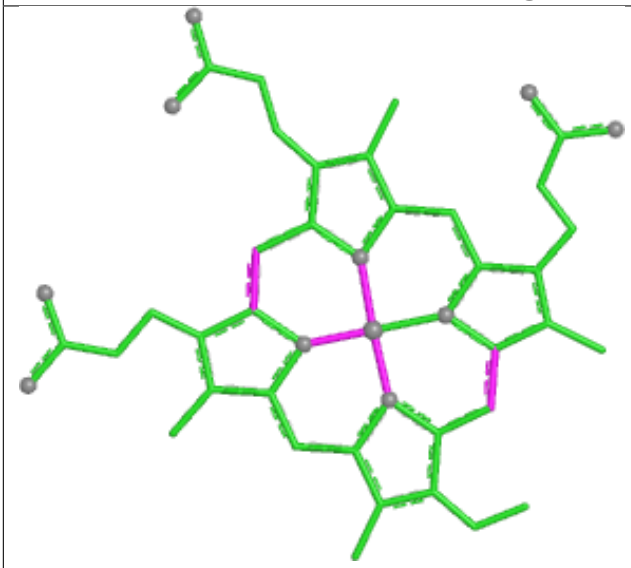


Torsions

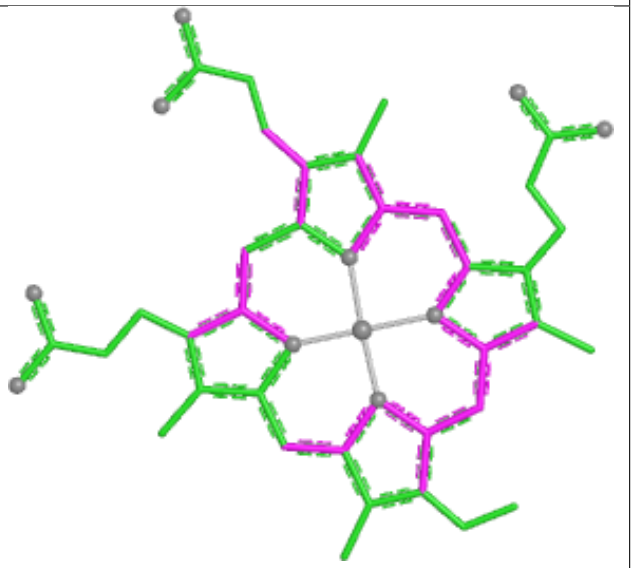


Rings

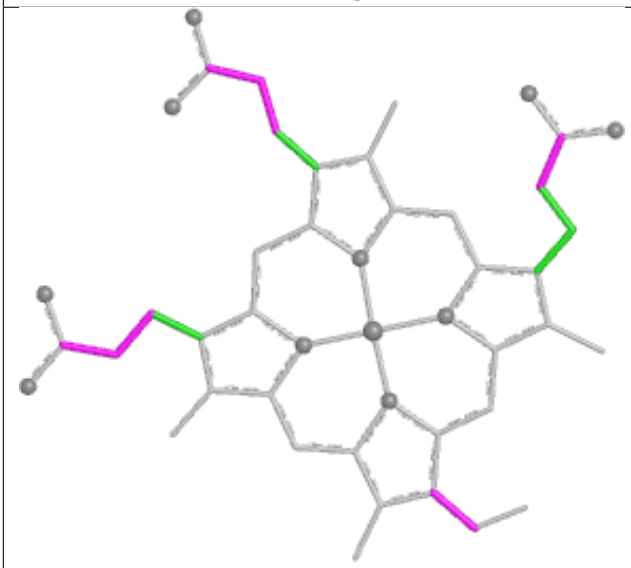
Ligand VOV G 301



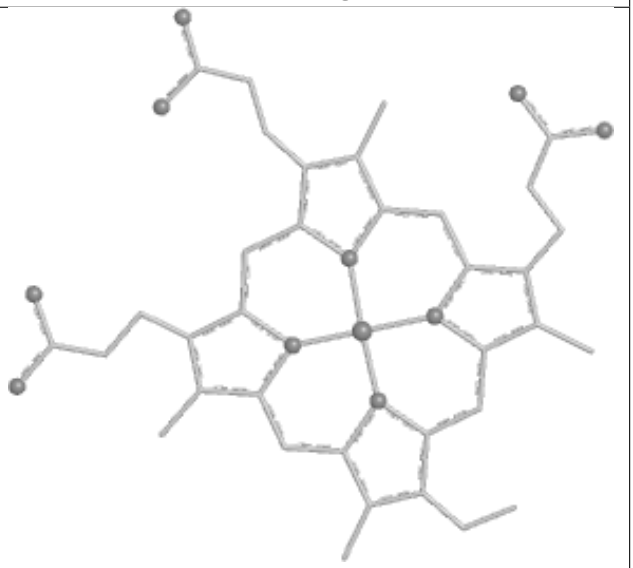
Bond lengths



Bond angles

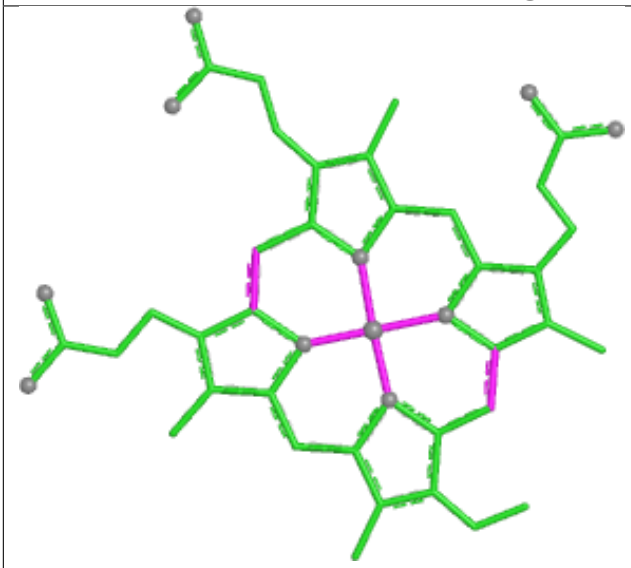


Torsions

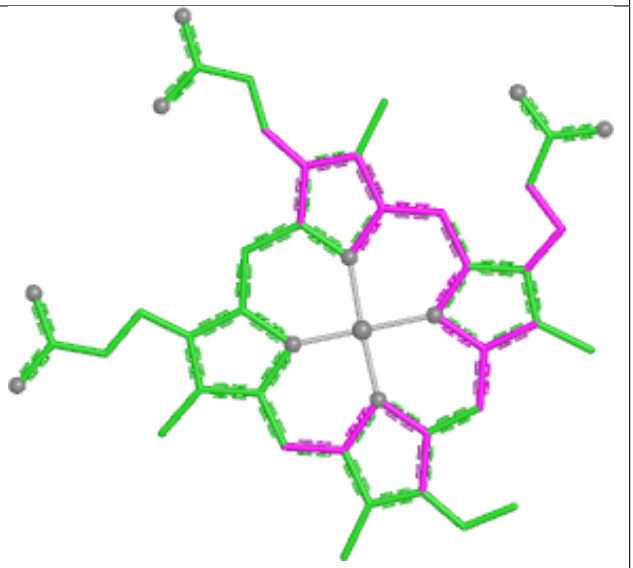


Rings

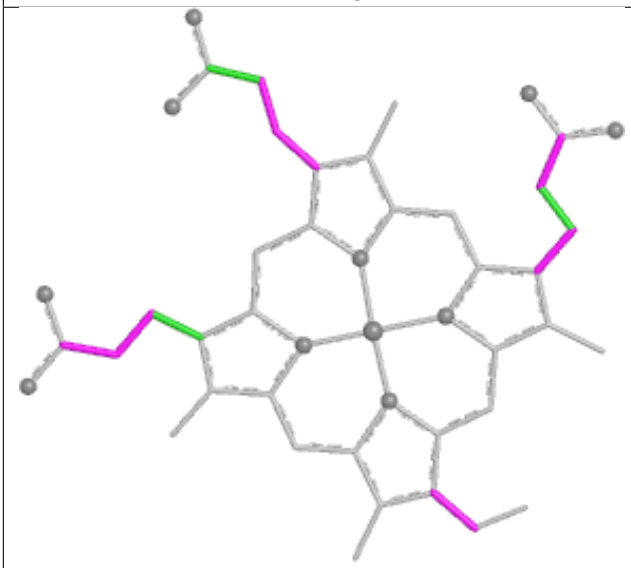
Ligand VOV A 301



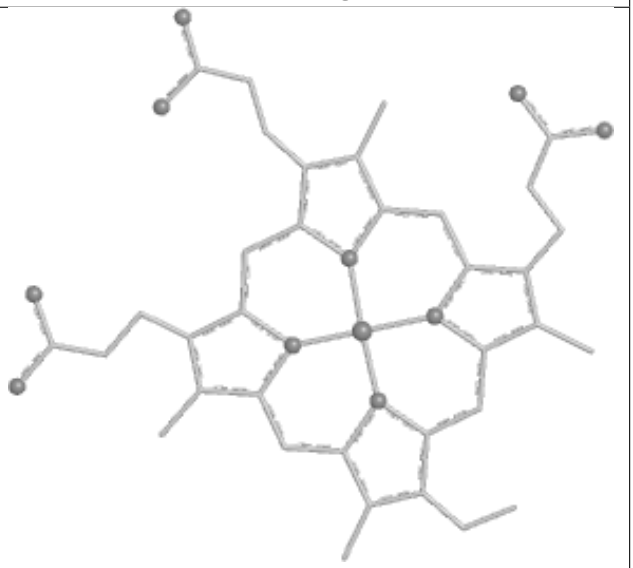
Bond lengths



Bond angles

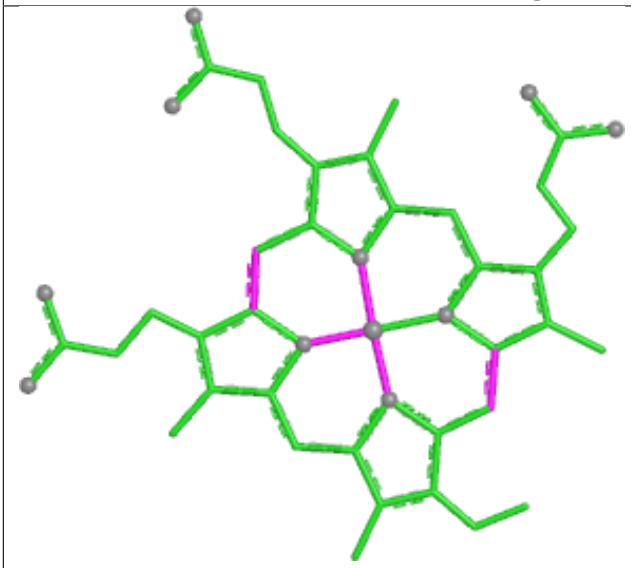


Torsions

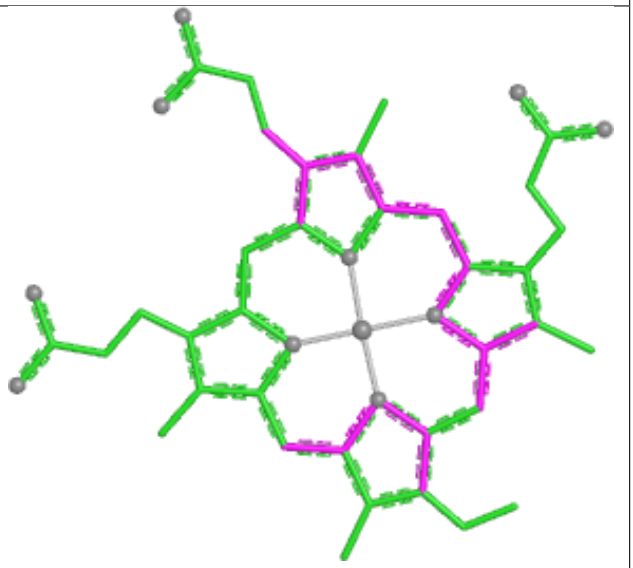


Rings

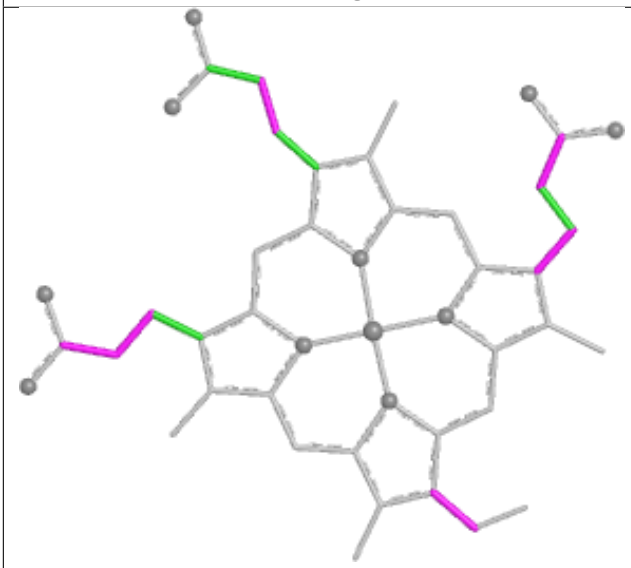
Ligand VOV I 301



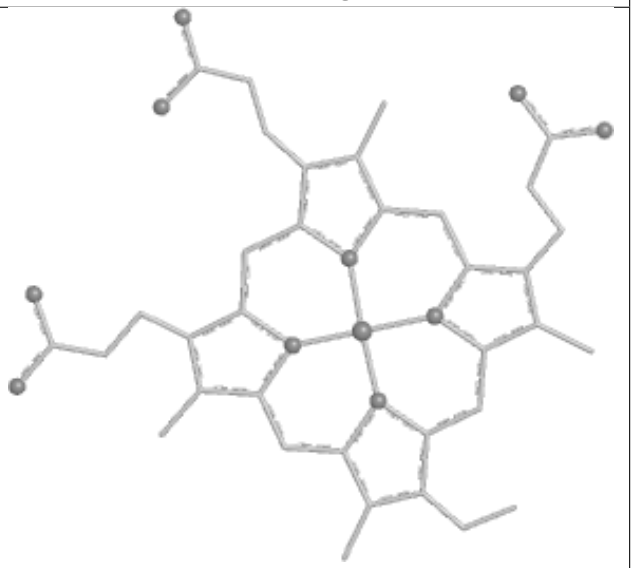
Bond lengths



Bond angles

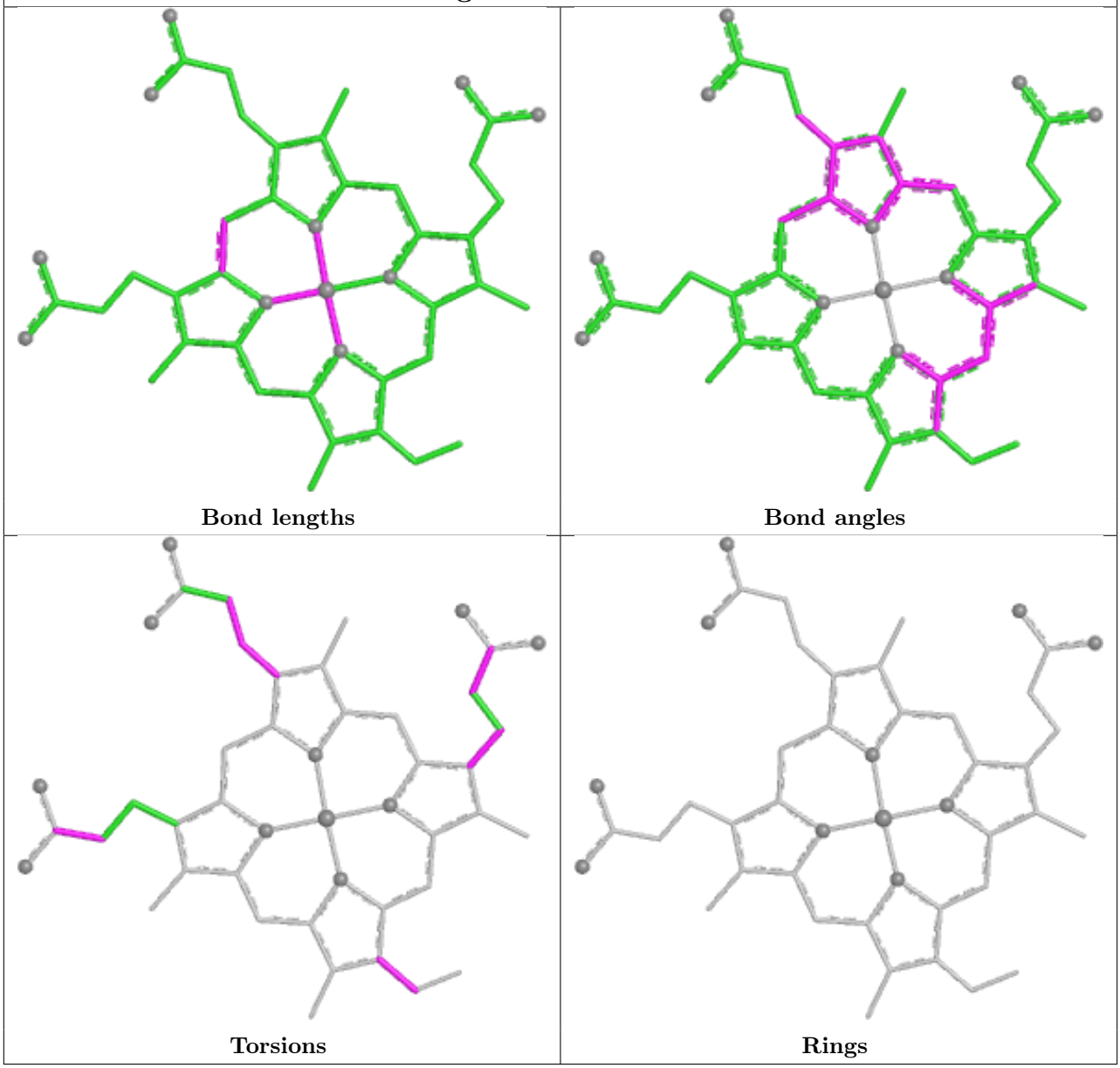


Torsions

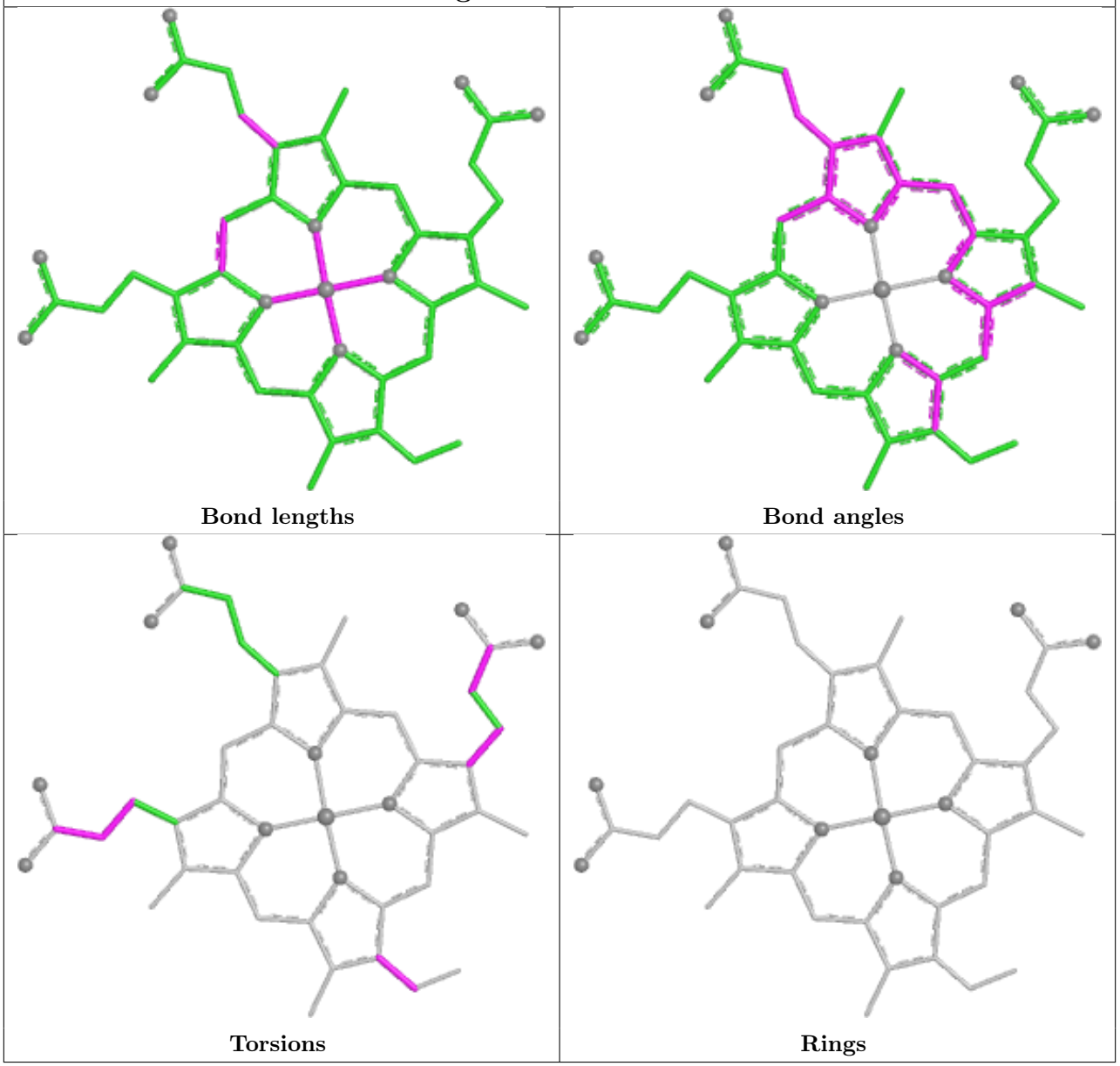


Rings

Ligand VOV B 301



Ligand VOV C 301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	221/243 (90%)	0.58	7 (3%) 50 46	46, 72, 95, 109	0
1	B	222/243 (91%)	-0.06	1 (0%) 87 85	40, 58, 75, 88	0
1	C	221/243 (90%)	0.34	3 (1%) 73 70	47, 66, 86, 102	0
1	D	222/243 (91%)	-0.14	0 100 100	41, 57, 74, 89	0
1	E	218/243 (89%)	-0.10	2 (0%) 81 78	41, 58, 76, 97	0
1	F	221/243 (90%)	0.27	4 (1%) 67 64	44, 69, 90, 108	0
1	G	222/243 (91%)	0.03	1 (0%) 87 85	42, 60, 82, 102	0
1	H	221/243 (90%)	0.40	5 (2%) 61 57	45, 66, 88, 104	0
1	I	221/243 (90%)	0.42	7 (3%) 50 46	43, 69, 94, 111	0
1	J	222/243 (91%)	0.03	2 (0%) 81 78	43, 59, 79, 97	0
All	All	2211/2430 (90%)	0.18	32 (1%) 73 70	40, 63, 87, 111	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	26	VAL	4.7
1	I	23	LEU	4.3
1	J	43	GLU	3.8
1	A	23	LEU	3.7
1	C	23	LEU	3.7
1	J	23	LEU	3.7
1	I	26	VAL	3.5
1	H	242	LEU	3.5
1	H	47	GLY	3.0
1	F	23	LEU	3.0
1	A	26	VAL	3.0
1	I	137	THR	3.0
1	F	137	THR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	22	ASP	2.9
1	E	137	THR	2.9
1	A	235	ILE	2.7
1	C	30	THR	2.6
1	I	133	LEU	2.5
1	I	134	ALA	2.5
1	F	235	ILE	2.5
1	G	240	ALA	2.4
1	I	27	ILE	2.4
1	A	133	LEU	2.4
1	H	173	ARG	2.4
1	C	243	ALA	2.3
1	B	170	LYS	2.3
1	A	179	ARG	2.2
1	H	46	ALA	2.2
1	A	134	ALA	2.2
1	F	135	ASP	2.2
1	A	135	ASP	2.1
1	I	135	ASP	2.1

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, 95^{th} 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	VOV	A	301	46/46	0.91	0.15	64,83,94,98	0
2	VOV	I	301	46/46	0.92	0.14	61,78,91,93	0
2	VOV	F	301	46/46	0.94	0.12	59,76,85,87	0
2	VOV	G	301	46/46	0.94	0.11	51,64,69,70	0

Continued on next page...

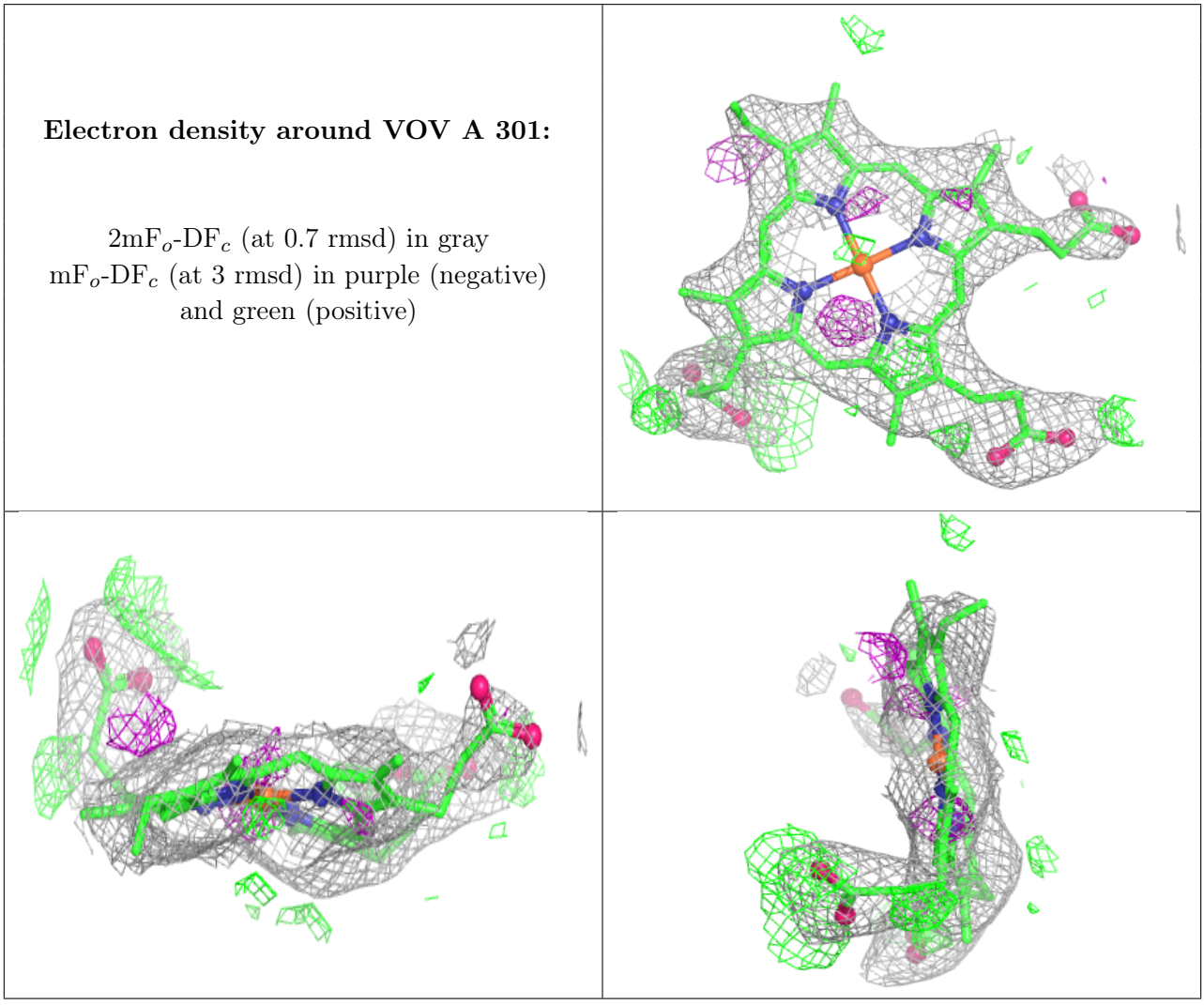
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	VOV	C	301	46/46	0.94	0.12	52,73,82,84	0
2	VOV	E	301	46/46	0.95	0.11	51,64,73,79	0
2	VOV	B	301	46/46	0.96	0.10	48,60,66,69	0
2	VOV	H	301	46/46	0.96	0.10	57,67,74,78	0
2	VOV	D	301	46/46	0.96	0.10	54,63,72,74	0
2	VOV	J	301	46/46	0.96	0.10	51,63,69,77	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.

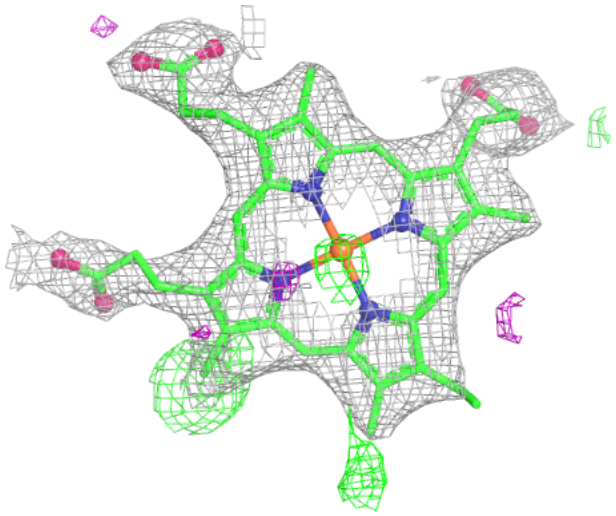
Electron density around VOV A 301:

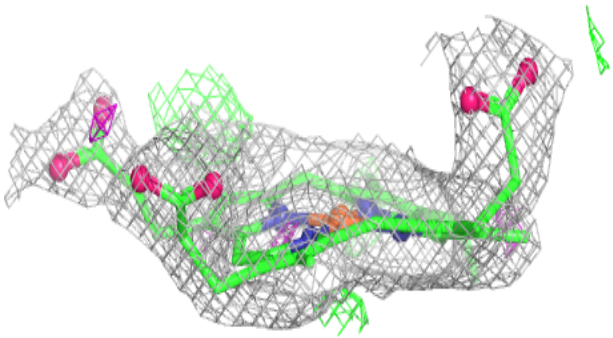
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

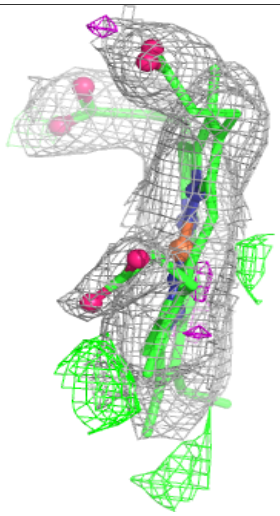


Electron density around VOV I 301:

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

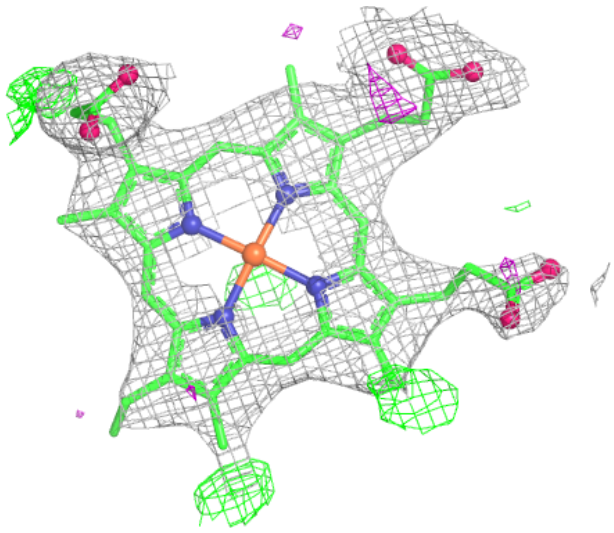


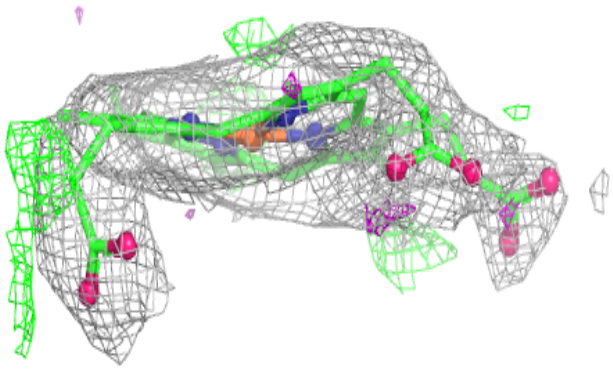


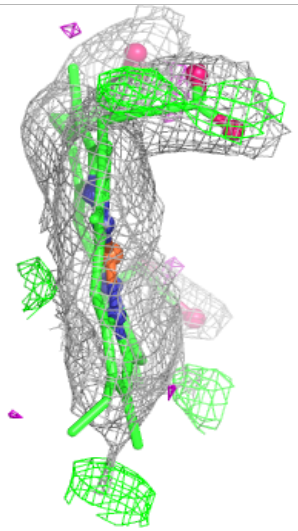


Electron density around VOV F 301:

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

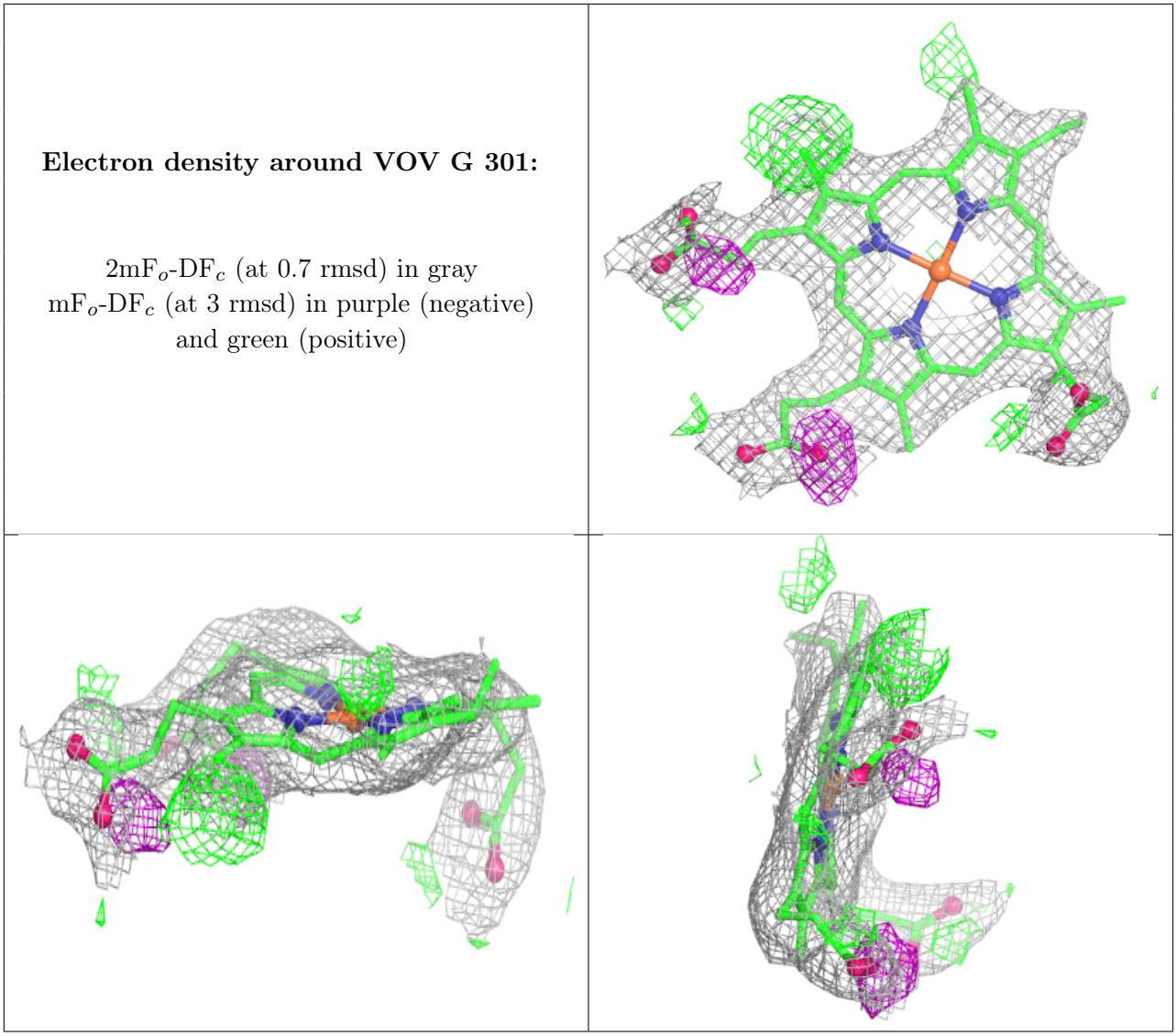






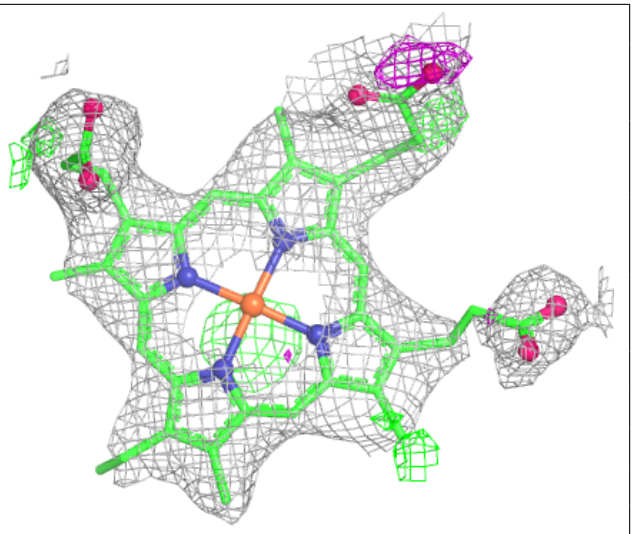
Electron density around VOV G 301:

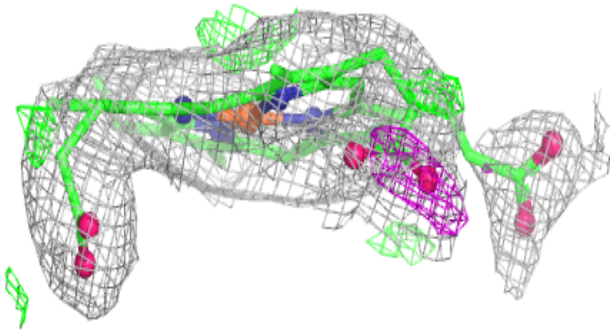
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

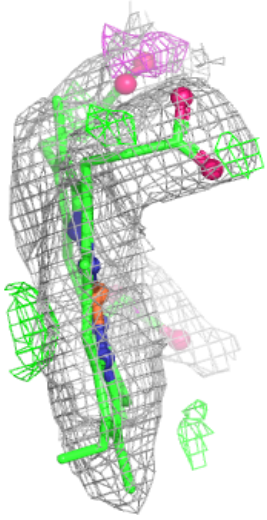


Electron density around VOV C 301:

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

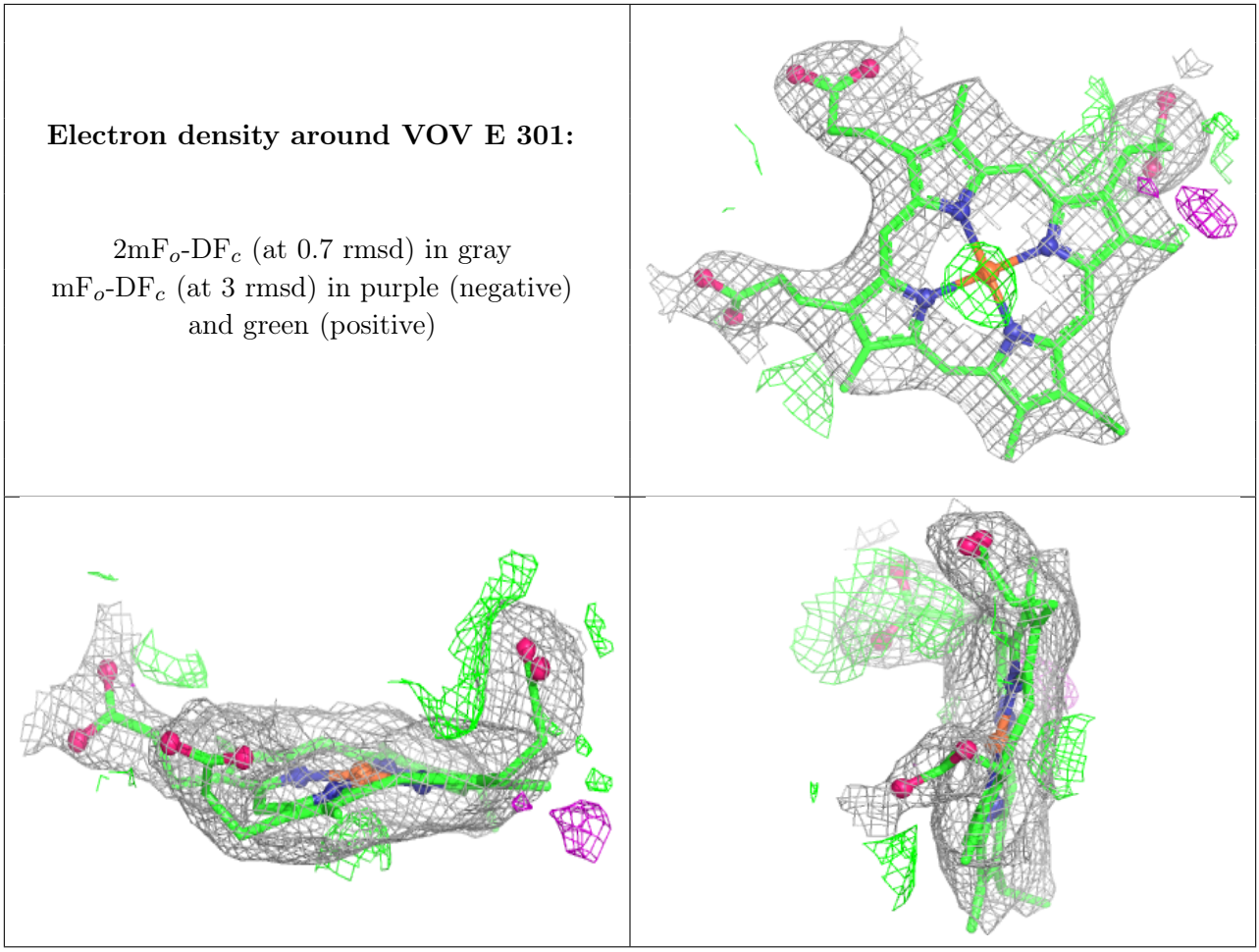






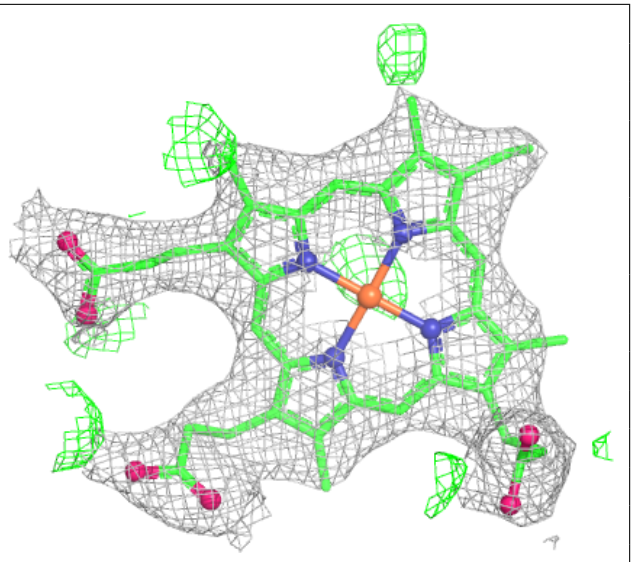
Electron density around VOV E 301:

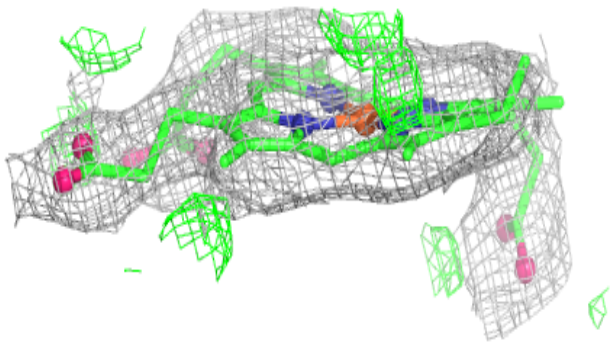
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

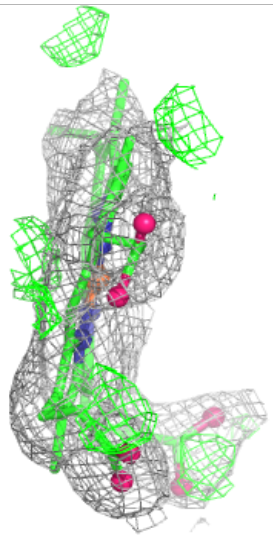


Electron density around VOV B 301:

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

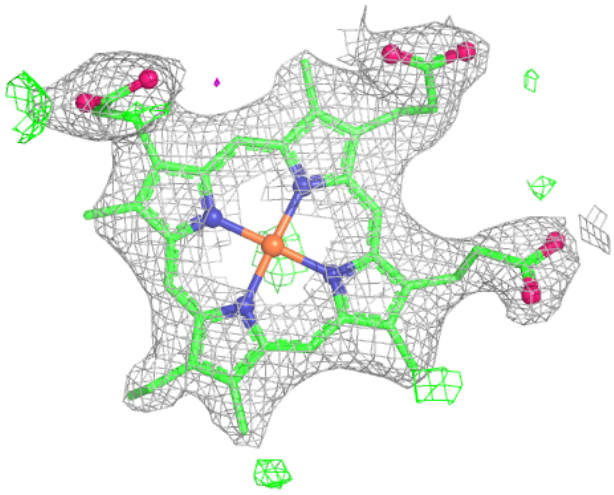


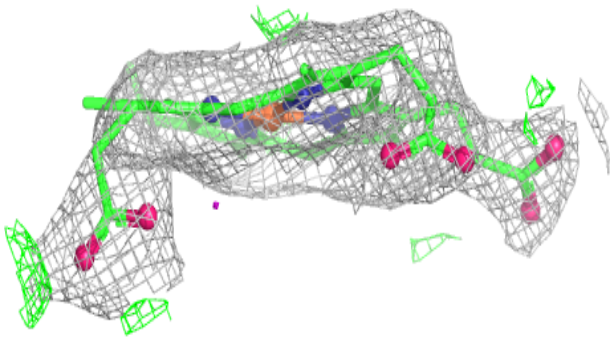


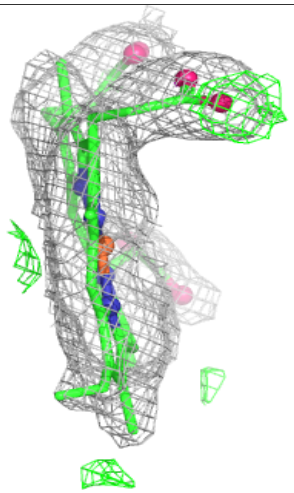


Electron density around VOV H 301:

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

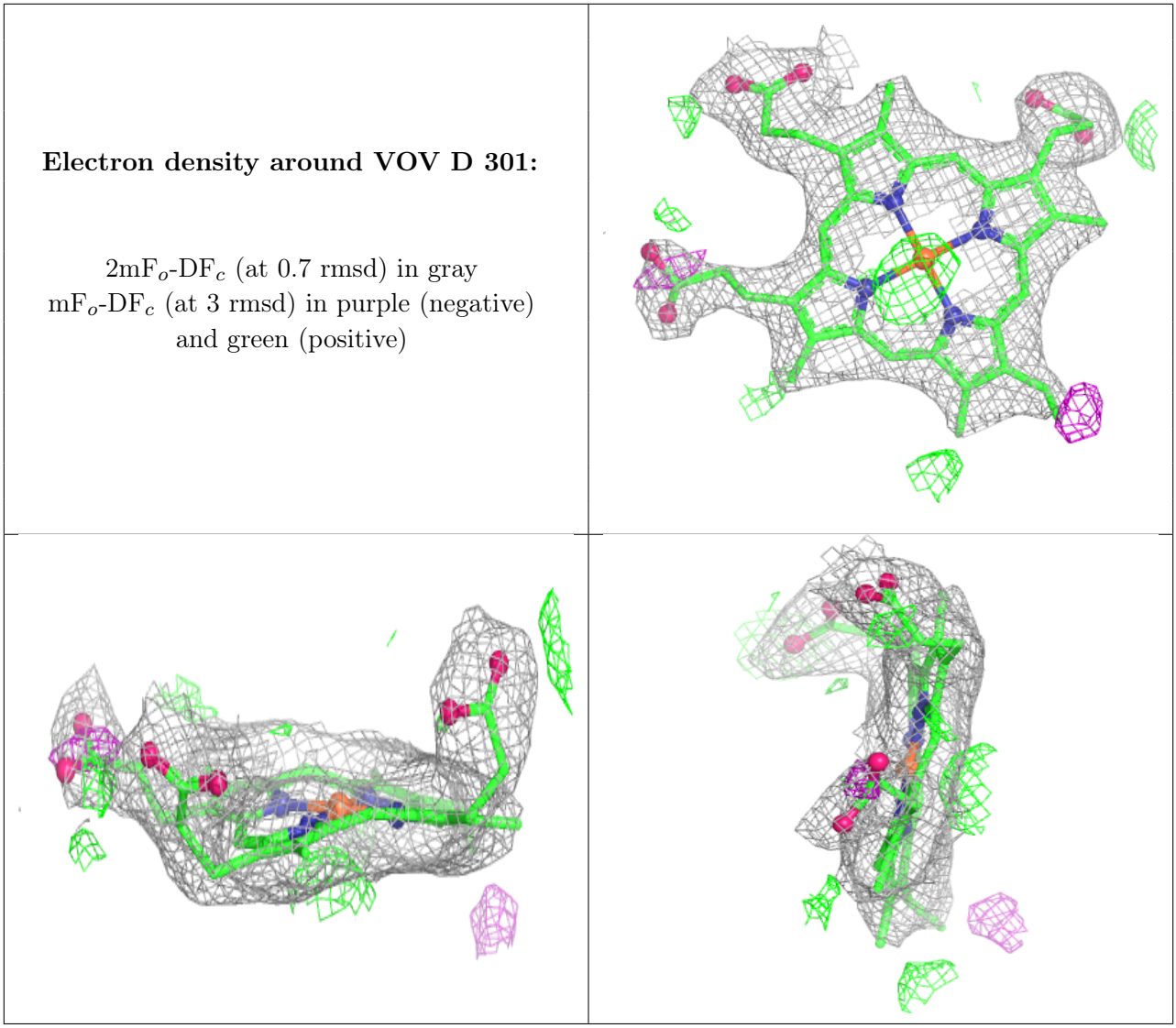






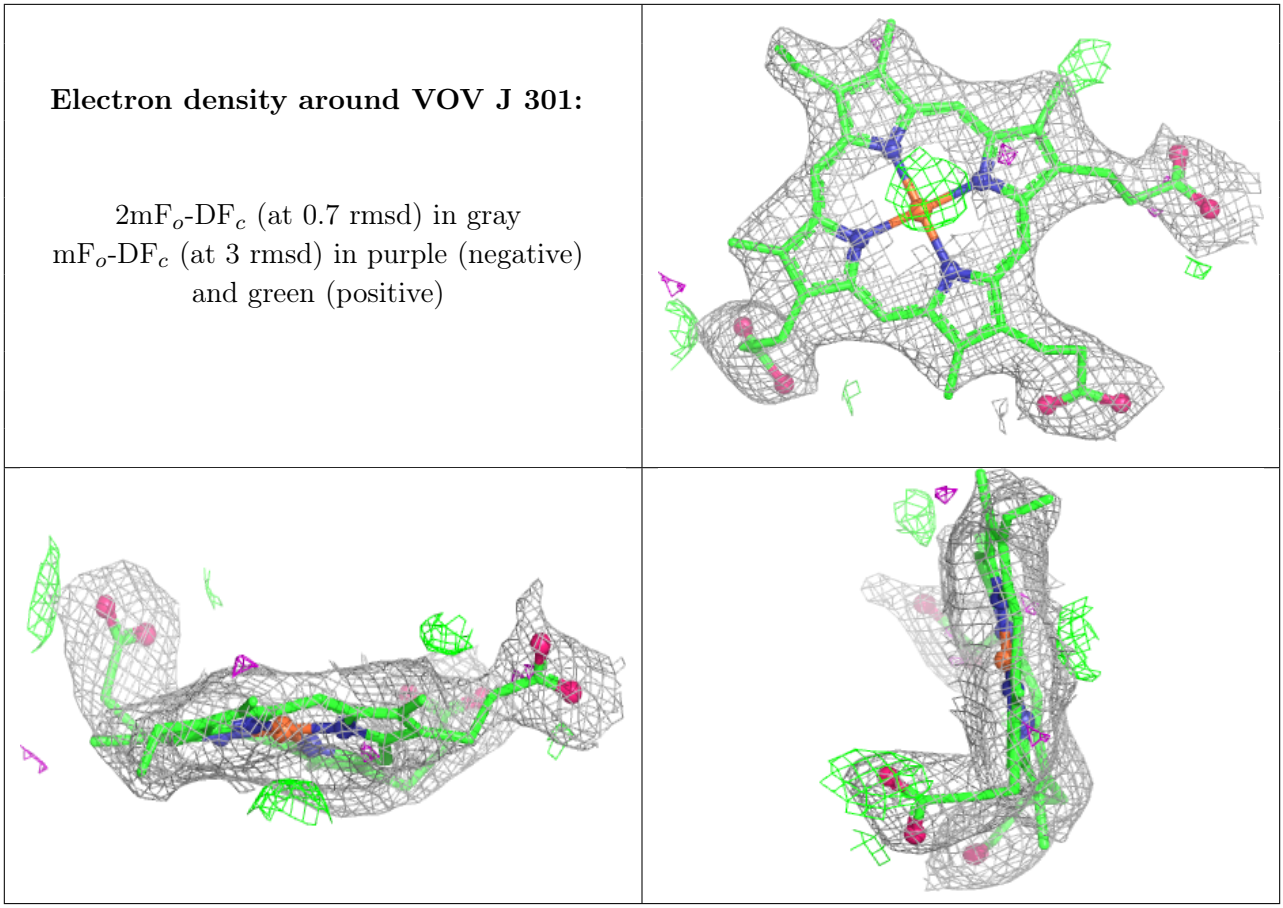
Electron density around VOV D 301:

$2mF_o$-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 J 301:

$2mF_o$-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.