Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2024 – 07:38 PM EDT

PDB ID	:	1NFV
Title	:	X-ray structure of Desulfovibrio desulfuricans bacterioferritin: the diiron centre in different catalytic states (as-isolated structure)
Authors	:	Macedo, S.; Romao, C.V.; Mitchell, E.; Matias, P.M.; Liu, M.Y.; Xavier, A.V.; LeGall, J.; Teixeira, M.; Lindley, P.; Carrondo, M.A.
Deposited on	:	2002-12-16
Resolution	:	1.95 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:

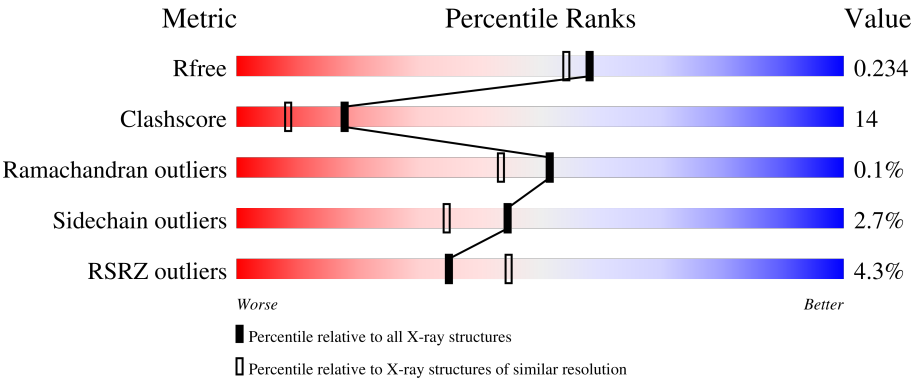
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	179	6% 75% 17% • 6%
1	B	179	5% 78% 15% • 5%
1	C	179	4% 72% 20% • 5%
1	D	179	5% 75% 17% •• 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	179	5% 78% 17% 5%
1	F	179	4% 77% 17% 5%
1	G	179	2% 81% 13% 6%
1	H	179	7% 78% 16% 5%
1	I	179	3% 78% 16% 5%
1	J	179	5% 82% 12% 5%
1	K	179	2% 83% 11% 5%
1	L	179	2% 77% 17% 5%
1	M	179	4% 82% 13% 5%
1	N	179	3% 79% 15% 5%
1	O	179	3% 78% 16% 6%
1	P	179	4% 74% 20% 5%

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
3	SO4	A	1004	-	-	-	X
3	SO4	A	1105	-	-	X	-
3	SO4	F	1502	-	-	X	-
3	SO4	G	1603	-	-	-	X
3	SO4	H	1703	-	-	-	X
3	SO4	I	1802	-	-	X	-
3	SO4	J	1906	-	-	X	-
3	SO4	L	2102	-	-	X	-
3	SO4	M	2206	-	-	X	-
3	SO4	O	2409	-	-	-	X
4	GOL	A	1010	-	X	-	-
4	GOL	B	1011	-	X	-	-
4	GOL	B	1110	-	X	-	-
4	GOL	C	1210	-	X	-	-
4	GOL	D	1211	-	X	X	-
4	GOL	E	1410	-	X	X	-
4	GOL	E	1411	-	X	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	F	1510	-	X	-	-
4	GOL	F	1512	-	X	-	-
4	GOL	G	1610	-	X	-	-
4	GOL	G	1611	-	X	-	-
4	GOL	H	1710	-	X	-	-
4	GOL	H	1814	-	X	-	-
4	GOL	I	1713	-	X	-	-
4	GOL	I	1810	-	X	X	-
4	GOL	J	1811	-	X	-	-
4	GOL	J	1910	-	X	X	-
4	GOL	K	2011	-	X	-	-
4	GOL	M	2210	-	X	X	-
4	GOL	M	2211	-	X	-	-
4	GOL	N	2310	-	X	-	-
4	GOL	O	2410	-	X	-	-
4	GOL	O	2411	-	X	-	-
4	GOL	P	2510	-	X	-	-
6	3PY	D	1310	-	X	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 25080 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.

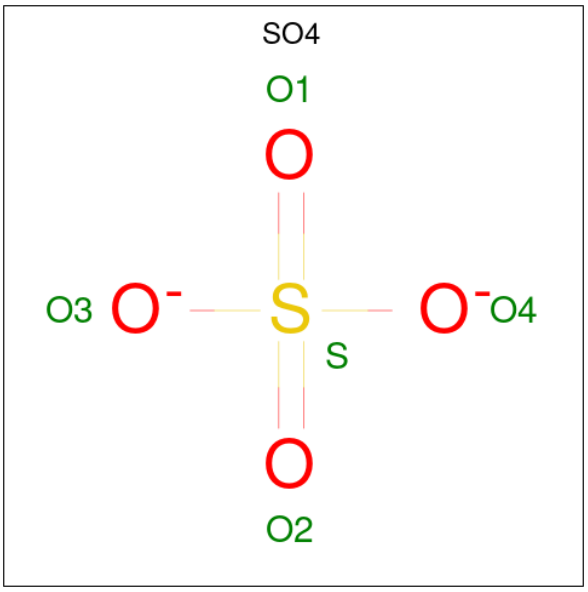
- Molecule 1 is a protein called bacterioferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	4	0
			1365	848	239	272	6			
1	B	170	Total	C	N	O	S	0	5	0
			1378	856	242	274	6			
1	C	170	Total	C	N	O	S	0	4	0
			1361	845	236	274	6			
1	D	170	Total	C	N	O	S	0	6	0
			1383	858	243	276	6			
1	E	170	Total	C	N	O	S	0	5	0
			1374	852	240	276	6			
1	F	170	Total	C	N	O	S	0	4	0
			1365	848	240	271	6			
1	G	169	Total	C	N	O	S	0	6	0
			1380	856	243	275	6			
1	H	170	Total	C	N	O	S	0	5	0
			1374	853	241	274	6			
1	I	170	Total	C	N	O	S	0	5	0
			1382	858	242	276	6			
1	J	170	Total	C	N	O	S	0	4	0
			1369	851	241	271	6			
1	K	170	Total	C	N	O	S	0	5	0
			1378	855	241	276	6			
1	L	170	Total	C	N	O	S	0	5	0
			1374	853	242	273	6			
1	M	170	Total	C	N	O	S	0	4	0
			1373	853	241	273	6			
1	N	170	Total	C	N	O	S	0	4	0
			1369	850	240	273	6			
1	O	169	Total	C	N	O	S	0	5	0
			1366	847	239	274	6			
1	P	170	Total	C	N	O	S	0	5	0
			1378	855	241	276	6			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Fe 2 2	0	0
2	B	2	Total Fe 2 2	0	0
2	C	2	Total Fe 2 2	0	0
2	D	2	Total Fe 2 2	0	0
2	E	2	Total Fe 2 2	0	0
2	F	2	Total Fe 2 2	0	0
2	G	2	Total Fe 2 2	0	0
2	H	2	Total Fe 2 2	0	0
2	I	2	Total Fe 2 2	0	0
2	J	2	Total Fe 2 2	0	0
2	K	2	Total Fe 2 2	0	0
2	L	2	Total Fe 2 2	0	0
2	M	2	Total Fe 2 2	0	0
2	N	2	Total Fe 2 2	0	0
2	O	2	Total Fe 2 2	0	0
2	P	2	Total Fe 2 2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

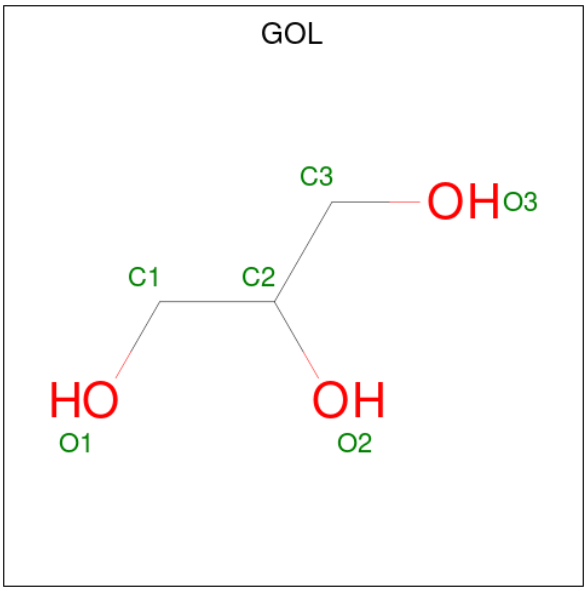
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	K	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		
3	M	1	Total	O	S	0	0
			5	4	1		
3	M	1	Total	O	S	0	0
			5	4	1		
3	N	1	Total	O	S	0	0
			5	4	1		
3	N	1	Total	O	S	0	0
			5	4	1		
3	N	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	P	1	Total	O	S	0	0
			5	4	1		
3	P	1	Total	O	S	0	0
			5	4	1		
3	P	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



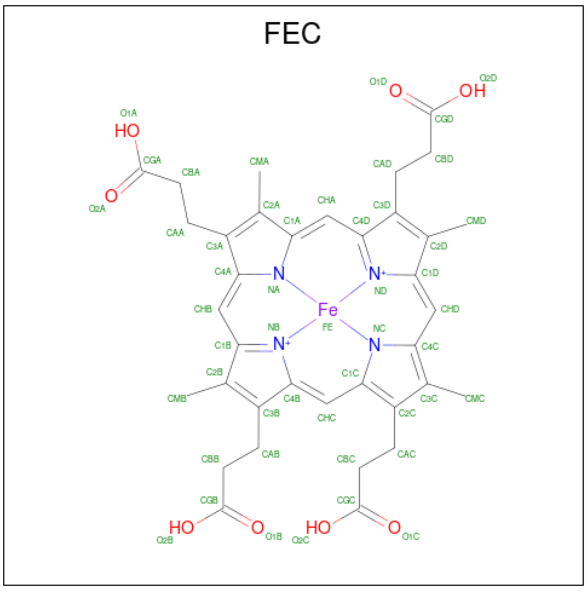
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	1	Total C O 6 3 3	0	0
4	J	1	Total C O 6 3 3	0	0
4	J	1	Total C O 6 3 3	0	0
4	K	1	Total C O 6 3 3	0	0
4	M	1	Total C O 6 3 3	0	0
4	M	1	Total C O 6 3 3	0	0
4	N	1	Total C O 6 3 3	0	0
4	O	1	Total C O 6 3 3	0	0
4	O	1	Total C O 6 3 3	0	0
4	P	1	Total C O 6 3 3	0	0

- Molecule 5 is 1,3,5,8-TETRAMETHYL-PORPHINE-2,4,6,7-TETRAPROPIONIC ACID FERROUS COMPLEX (three-letter code: FEC) (formula: $C_{36}H_{36}FeN_4O_8$).



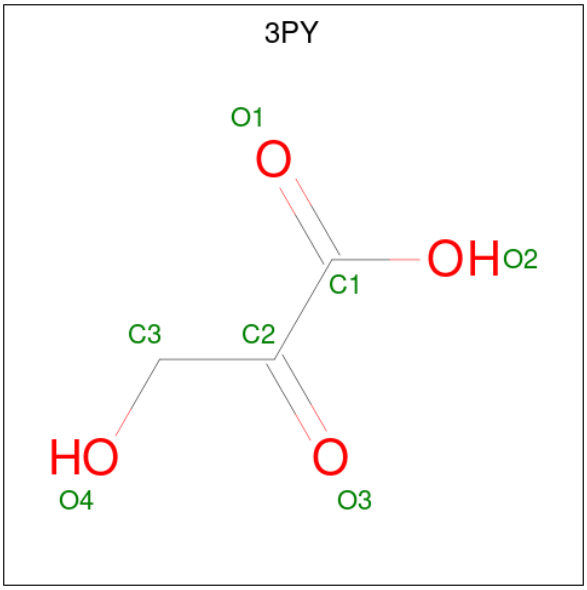
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C Fe N O 98 72 2 8 16	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	Fe	N	O	0	1
			98	72	2	8	16		
5	F	1	Total	C	Fe	N	O	0	1
			98	72	2	8	16		
5	G	1	Total	C	Fe	N	O	0	1
			98	72	2	8	16		
5	I	1	Total	C	Fe	N	O	0	1
			98	72	2	8	16		
5	L	1	Total	C	Fe	N	O	0	1
			98	72	2	8	16		
5	M	1	Total	C	Fe	N	O	0	1
			98	72	2	8	16		
5	P	1	Total	C	Fe	N	O	0	1
			98	72	2	8	16		

- Molecule 6 is 3-HYDROXYPYRUVIC ACID (three-letter code: 3PY) (formula: $C_3H_4O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	131	Total	O	0	0
			131	131		

Continued on next page...

Continued from previous page...

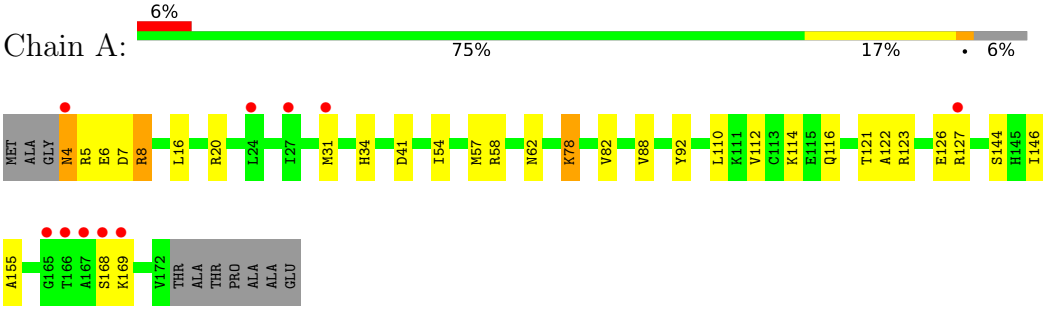
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	142	Total O 142 142	0	0
7	C	117	Total O 117 117	0	0
7	D	99	Total O 99 99	0	0
7	E	101	Total O 101 101	0	0
7	F	103	Total O 103 103	0	0
7	G	146	Total O 146 146	0	0
7	H	91	Total O 91 91	0	0
7	I	131	Total O 131 131	0	0
7	J	99	Total O 99 99	0	0
7	K	130	Total O 130 130	0	0
7	L	134	Total O 134 134	0	0
7	M	122	Total O 122 122	0	0
7	N	124	Total O 124 124	0	0
7	O	105	Total O 105 105	0	0
7	P	115	Total O 115 115	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.

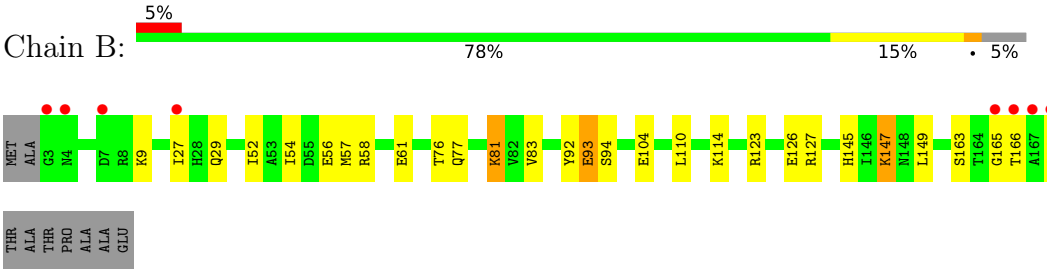
• Molecule 1: bacterioferritin

Chain A:



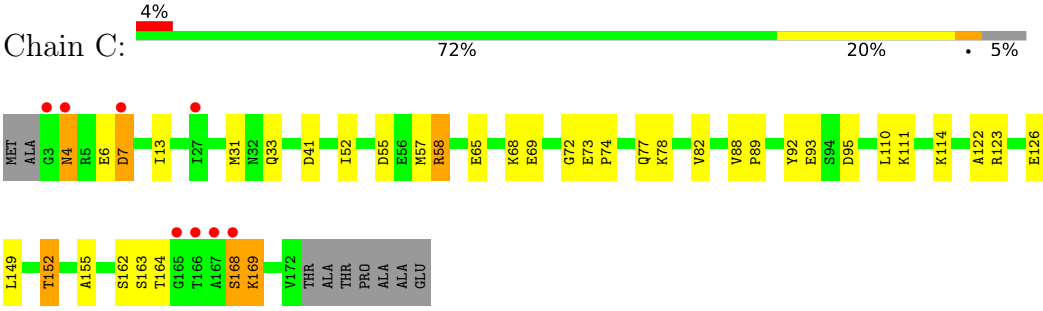
• Molecule 1: bacterioferritin

Chain B:



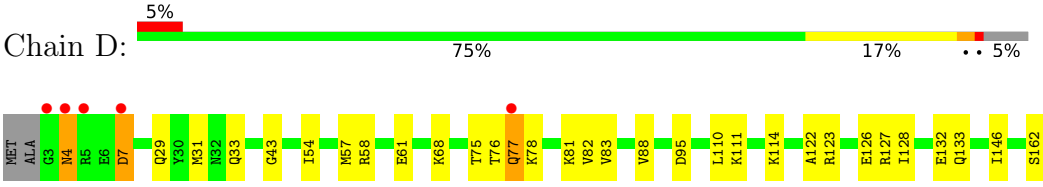
• Molecule 1: bacterioferritin

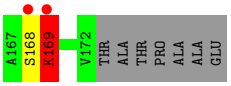
Chain C:



• Molecule 1: bacterioferritin

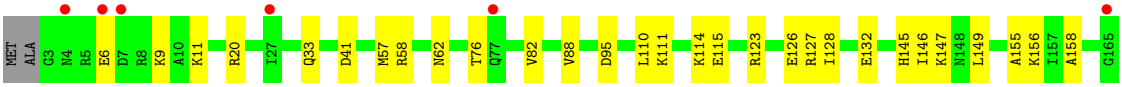
Chain D:

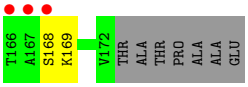




• Molecule 1: bacterioferritin

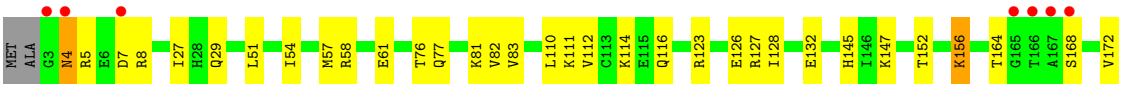
Chain E:





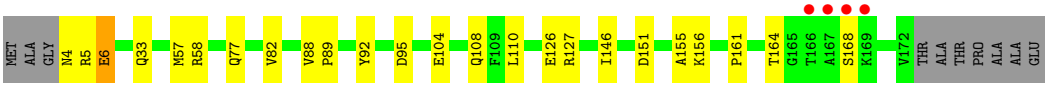
• Molecule 1: bacterioferritin

Chain F:



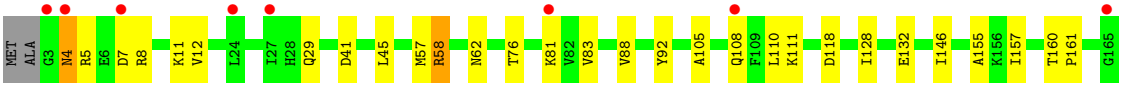
• Molecule 1: bacterioferritin

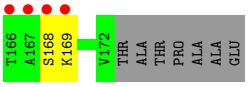
Chain G:



• Molecule 1: bacterioferritin

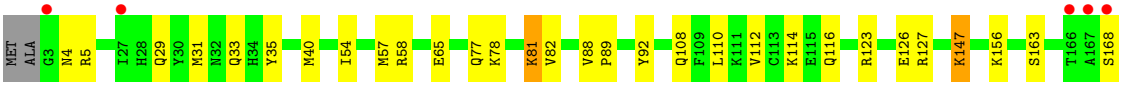
Chain H:

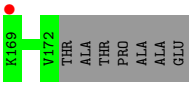




• Molecule 1: bacterioferritin

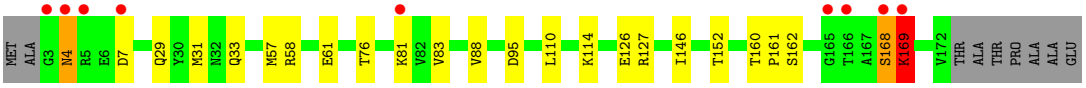
Chain I:





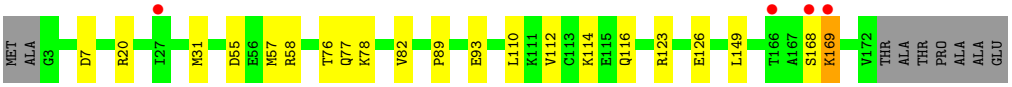
• Molecule 1: bacterioferritin

Chain J:



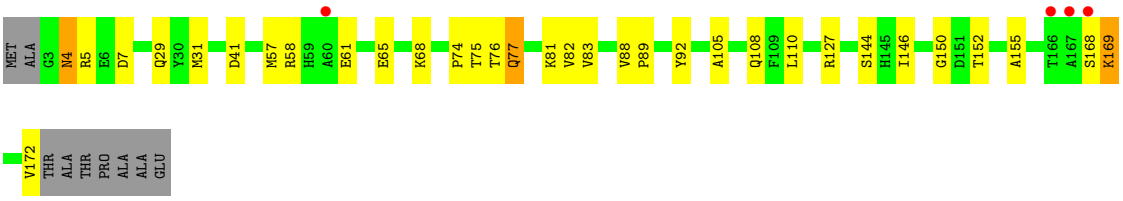
• Molecule 1: bacterioferritin

Chain K:



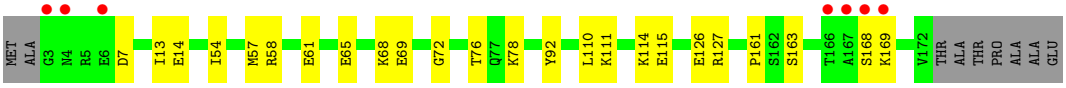
• Molecule 1: bacterioferritin

Chain L:



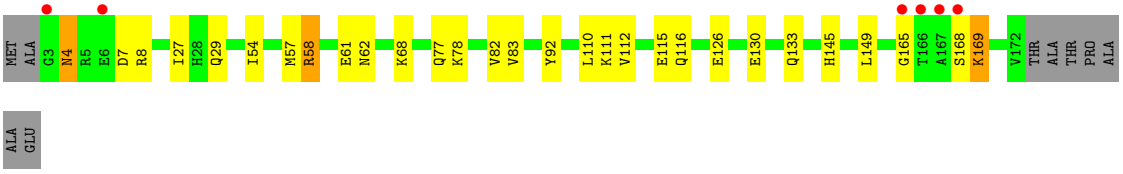
• Molecule 1: bacterioferritin

Chain M:



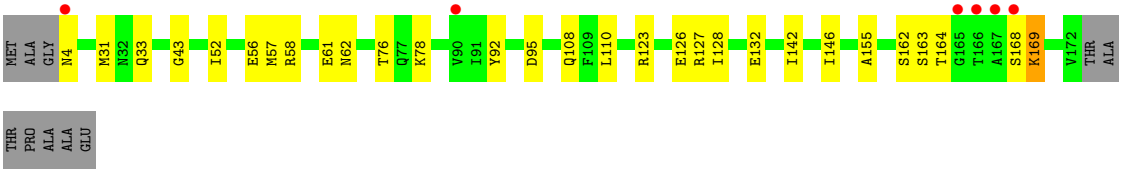
• Molecule 1: bacterioferritin

Chain N:

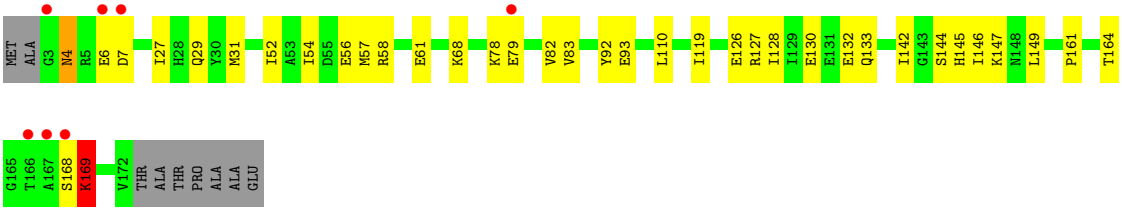


• Molecule 1: bacterioferritin

Chain O:



• Molecule 1: bacterioferritin



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	225.30Å 225.30Å 225.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.95 29.84 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.9 (30.00-1.95) 99.2 (29.84-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 1.95Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.214 , 0.254 0.185 , 0.234	Depositor DCC
R_{free} test set	5260 reflections (1.94%)	wwPDB-VP
Wilson B-factor (Å^2)	27.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 60.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	25080	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.35% 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, 3PY, GOL, FE, SO4

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	0.31	0/1385	0.93	3/1864 (0.2%)
1	B	0.31	0/1398	0.84	1/1880 (0.1%)
1	C	0.32	0/1381	0.89	3/1861 (0.2%)
1	D	0.51	2/1407 (0.1%)	0.86	0/1892
1	E	0.31	0/1398	0.84	1/1881 (0.1%)
1	F	0.31	0/1389	0.83	0/1868
1	G	0.44	2/1405 (0.1%)	0.91	1/1890 (0.1%)
1	H	0.32	0/1394	0.85	1/1876 (0.1%)
1	I	0.31	0/1402	0.86	1/1885 (0.1%)
1	J	0.34	0/1389	0.86	2/1868 (0.1%)
1	K	0.32	0/1398	0.88	3/1881 (0.2%)
1	L	1.07	2/1398 (0.1%)	0.90	3/1880 (0.2%)
1	M	0.31	0/1393	0.84	1/1873 (0.1%)
1	N	0.30	0/1389	0.80	1/1869 (0.1%)
1	O	0.77	2/1390 (0.1%)	0.92	3/1872 (0.2%)
1	P	0.60	2/1402 (0.1%)	0.85	3/1885 (0.2%)
All	All	0.48	10/22318 (0.0%)	0.87	27/30025 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	169[A]	LYS	CB-CG	27.00	2.25	1.52
1	L	169[B]	LYS	CB-CG	27.00	2.25	1.52
1	O	169[A]	LYS	CB-CG	18.20	2.01	1.52
1	O	169[B]	LYS	CB-CG	18.20	2.01	1.52
1	P	169[A]	LYS	CB-CG	13.45	1.88	1.52
1	P	169[B]	LYS	CB-CG	13.45	1.88	1.52
1	D	169[A]	LYS	CB-CG	10.65	1.81	1.52
1	D	169[B]	LYS	CB-CG	10.65	1.81	1.52
1	G	6[A]	GLU	CD-OE1	5.97	1.32	1.25
1	G	6[B]	GLU	CD-OE1	5.97	1.32	1.25

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	169[A]	LYS	CA-CB-CG	-9.37	92.78	113.40
1	L	169[B]	LYS	CA-CB-CG	-9.37	92.78	113.40
1	O	169[A]	LYS	CA-CB-CG	-7.31	97.32	113.40
1	O	169[B]	LYS	CA-CB-CG	-7.31	97.32	113.40
1	C	58[A]	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	C	58[B]	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	K	20	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	E	123	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	L	92	TYR	CA-CB-CG	-5.88	102.24	113.40
1	A	20	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	O	92	TYR	CA-CB-CG	-5.71	102.54	113.40
1	P	169[A]	LYS	CA-CB-CG	-5.62	101.04	113.40
1	P	169[B]	LYS	CA-CB-CG	-5.62	101.04	113.40
1	I	92	TYR	CA-CB-CG	-5.57	102.81	113.40
1	H	92	TYR	CA-CB-CG	-5.56	102.83	113.40
1	M	92	TYR	CA-CB-CG	-5.44	103.06	113.40
1	N	92	TYR	CA-CB-CG	-5.37	103.20	113.40
1	J	169[A]	LYS	C-N-CA	5.33	133.48	122.30
1	J	169[B]	LYS	C-N-CA	5.33	133.48	122.30
1	G	92	TYR	CA-CB-CG	-5.20	103.53	113.40
1	A	92	TYR	CA-CB-CG	-5.19	103.54	113.40
1	C	92	TYR	CA-CB-CG	-5.19	103.54	113.40
1	K	123	ARG	CD-NE-CZ	5.17	130.85	123.60
1	K	123	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	8	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	P	92	TYR	CA-CB-CG	-5.03	103.84	113.40
1	B	92	TYR	CA-CB-CG	-5.03	103.85	113.40

There are no chirality outliers.

There are no planarity outliers.

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	1365	0	1325	44	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1378	0	1343	43	0
1	C	1361	0	1312	51	0
1	D	1383	0	1341	55	0
1	E	1374	0	1326	37	0
1	F	1365	0	1328	37	0
1	G	1380	0	1340	43	0
1	H	1374	0	1332	35	0
1	I	1382	0	1348	53	0
1	J	1369	0	1335	34	0
1	K	1378	0	1335	32	0
1	L	1374	0	1335	35	0
1	M	1373	0	1341	54	0
1	N	1369	0	1329	56	0
1	O	1366	0	1312	46	0
1	P	1378	0	1338	47	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
2	O	2	0	0	0	0
2	P	2	0	0	0	0
3	A	25	0	0	3	0
3	B	20	0	0	3	0
3	C	15	0	0	2	0
3	D	10	0	0	0	0
3	E	15	0	0	1	0
3	F	15	0	0	3	0
3	G	15	0	0	1	0
3	H	15	0	0	0	0
3	I	20	0	0	2	7
3	J	15	0	0	4	0
3	K	20	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	20	0	0	3	7
3	M	10	0	0	2	0
3	N	15	0	0	0	0
3	O	10	0	0	2	0
3	P	15	0	0	2	0
4	A	6	0	4	1	0
4	B	12	0	8	3	0
4	C	6	0	5	0	0
4	D	6	0	4	5	0
4	E	12	0	8	6	0
4	F	12	0	8	3	0
4	G	12	0	9	3	0
4	H	12	0	8	1	0
4	I	12	0	8	16	0
4	J	12	0	8	5	0
4	K	6	0	4	1	0
4	M	12	0	8	8	0
4	N	6	0	4	1	0
4	O	12	0	8	4	0
4	P	6	0	4	2	0
5	B	98	0	64	17	0
5	D	98	0	64	22	0
5	F	98	0	64	17	0
5	G	98	0	64	15	0
5	I	98	0	64	18	0
5	L	98	0	64	23	0
5	M	98	0	64	18	0
5	P	98	0	64	21	0
6	D	6	0	1	1	0
7	A	131	0	0	6	0
7	B	142	0	0	5	0
7	C	117	0	0	0	0
7	D	99	0	0	9	0
7	E	101	0	0	2	0
7	F	103	0	0	2	0
7	G	146	0	0	5	0
7	H	91	0	0	0	0
7	I	131	0	0	5	0
7	J	99	0	0	5	0
7	K	130	0	0	4	0
7	L	134	0	0	5	0
7	M	122	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	N	124	0	0	1	0
7	O	105	0	0	5	0
7	P	115	0	0	5	0
All	All	25080	0	21931	603	7

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 14.

All (603) 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:M:168[A]:SER:CB	1:N:58[A]:ARG:HH22	1.00	1.53
1:G:168[A]:SER:CB	1:H:58[A]:ARG:HH22	1.23	1.49
1:O:58[B]:ARG:NH2	1:P:168[B]:SER:H	1.15	1.44
1:M:168[A]:SER:HB2	1:N:58[A]:ARG:NH2	1.32	1.44
1:G:168[A]:SER:HB2	1:H:58[A]:ARG:NH2	1.12	1.41
1:O:58[B]:ARG:NH2	1:P:168[B]:SER:N	1.66	1.40
1:M:168[A]:SER:CB	1:N:58[A]:ARG:NH2	1.81	1.35
1:I:127[A]:ARG:HD3	4:I:1810:GOL:O1	1.15	1.29
1:L:168[A]:SER:HA	5:L:2108[A]:FEC:O2C	1.21	1.28
1:G:168[A]:SER:CB	1:H:58[A]:ARG:NH2	1.88	1.20
1:K:168[B]:SER:HA	5:L:2108[B]:FEC:O2C	1.42	1.16
1:O:58[B]:ARG:NH2	1:P:168[B]:SER:CA	2.10	1.15
1:G:6[A]:GLU:OE1	7:G:1620:HOH:O	1.61	1.14
1:I:127[B]:ARG:HG2	4:I:1810:GOL:O1	1.47	1.11
1:K:168[A]:SER:O	1:L:58[A]:ARG:NH2	1.86	1.09
1:O:168[A]:SER:O	1:P:58[A]:ARG:NH2	1.84	1.09
1:E:168[B]:SER:O	1:F:58[B]:ARG:NH2	1.87	1.07
5:M:2207[B]:FEC:HBC1	1:N:168[B]:SER:OG	0.88	1.06
1:C:168[A]:SER:O	1:D:58[A]:ARG:NH2	1.91	1.03
1:O:58[B]:ARG:NH2	1:P:168[B]:SER:CB	2.23	1.00
1:I:127[A]:ARG:CD	4:I:1810:GOL:HO1	1.71	0.99
1:A:78:LYS:HE2	3:A:1105:SO4:O3	1.63	0.98
1:I:127[B]:ARG:CD	4:I:1810:GOL:O1	2.11	0.98
1:O:168[B]:SER:HA	5:P:2507[B]:FEC:O2C	0.80	0.97
1:G:168[A]:SER:CA	1:H:58[A]:ARG:NH2	2.30	0.95
1:N:110:LEU:HD11	1:N:126:GLU:HG3	1.49	0.95
1:M:168[A]:SER:CA	1:N:58[A]:ARG:HH22	1.78	0.94
1:E:168[B]:SER:C	1:F:58[B]:ARG:NH2	2.21	0.94
1:C:58[B]:ARG:NH2	1:D:168[B]:SER:CB	2.30	0.94
1:I:127[A]:ARG:HB3	4:I:1810:GOL:O1	1.67	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:168[B]:SER:CB	5:L:2108[B]:FEC:O2C	2.17	0.93
1:L:168[A]:SER:HB3	5:L:2108[A]:FEC:O2C	1.69	0.90
1:H:29:GLN:HE22	1:H:83:VAL:H	1.20	0.90
1:L:168[A]:SER:HA	5:L:2108[A]:FEC:CGC	2.03	0.89
1:C:58[B]:ARG:NH2	1:D:168[B]:SER:HB2	1.88	0.89
1:C:58[B]:ARG:NH2	1:D:168[B]:SER:CA	2.35	0.89
1:G:168[A]:SER:CA	1:H:58[A]:ARG:HH21	1.86	0.88
1:O:168[A]:SER:HB2	1:P:58[A]:ARG:HH12	1.38	0.88
1:J:110:LEU:HD11	1:J:126:GLU:HG3	1.56	0.87
1:M:168[A]:SER:CA	1:N:58[A]:ARG:NH2	2.37	0.87
5:G:1608[B]:FEC:HBC2	5:G:1608[B]:FEC:HHC	1.58	0.86
1:I:127[A]:ARG:CB	4:I:1810:GOL:O1	2.24	0.86
1:C:147:LYS:NZ	3:C:1203:SO4:O4	2.08	0.86
1:D:29:GLN:HE22	1:D:83:VAL:H	1.20	0.86
5:D:1311[A]:FEC:HBC2	5:D:1311[A]:FEC:HHC	1.56	0.85
1:M:168[A]:SER:HB3	1:N:58[A]:ARG:NH2	1.91	0.85
5:B:1107[A]:FEC:HBC2	5:B:1107[A]:FEC:HHC	1.58	0.84
1:J:161:PRO:HA	3:J:1906:SO4:O1	1.77	0.84
1:K:169[B]:LYS:HB3	7:K:9227:HOH:O	1.79	0.82
3:F:1501:SO4:O2	7:F:660:HOH:O	1.97	0.82
1:D:110:LEU:HD11	1:D:126:GLU:HG2	1.63	0.81
1:G:168[A]:SER:N	1:H:58[A]:ARG:HH21	1.78	0.81
1:C:149:LEU:O	1:C:152[B]:THR:HG22	1.81	0.80
1:I:163:SER:HB3	7:I:9021:HOH:O	1.81	0.80
1:G:156:LYS:HD2	7:M:898:HOH:O	1.80	0.80
1:O:123:ARG:NH2	3:O:2409:SO4:O1	2.15	0.80
5:M:2207[B]:FEC:HBC1	1:N:168[B]:SER:CB	2.09	0.80
1:B:149:LEU:HD13	1:H:155:ALA:HA	1.64	0.80
1:J:168[B]:SER:HA	7:J:9964:HOH:O	1.81	0.79
1:M:168[A]:SER:HB2	1:N:58[A]:ARG:CZ	2.13	0.79
5:L:2108[A]:FEC:HHC	5:L:2108[A]:FEC:HBC2	1.63	0.79
1:M:168[A]:SER:HB2	1:N:58[A]:ARG:HH22	0.63	0.79
1:I:81:LYS:HE3	1:I:82:VAL:H	1.47	0.79
1:D:168[B]:SER:OG	5:D:1311[B]:FEC:CGC	2.30	0.79
1:C:58[B]:ARG:HH21	1:D:168[B]:SER:C	1.86	0.78
1:G:164:THR:HA	7:G:1691:HOH:O	1.82	0.78
1:D:168[B]:SER:OG	5:D:1311[B]:FEC:CBC	2.33	0.77
1:G:168[A]:SER:HB3	5:G:1608[A]:FEC:HBC1	1.67	0.77
1:F:29:GLN:HE22	1:F:83:VAL:H	1.29	0.77
1:H:105:ALA:HA	1:H:108:GLN:OE1	1.84	0.76
1:P:29:GLN:HE22	1:P:83:VAL:H	1.34	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:ASN:ND2	1:D:7:ASP:HB2	2.01	0.76
1:I:110:LEU:HD23	1:I:114:LYS:HD2	1.66	0.76
3:F:1502:SO4:O2	7:F:680:HOH:O	2.03	0.75
1:I:127[A]:ARG:HD3	4:I:1810:GOL:HO1	0.94	0.75
1:J:169[A]:LYS:HB3	7:J:9004:HOH:O	1.87	0.75
1:L:168[B]:SER:OG	5:L:2108[B]:FEC:HAC2	1.86	0.74
1:O:168[A]:SER:OG	5:P:2507[A]:FEC:HAC2	1.87	0.74
1:E:127[B]:ARG:HB3	4:E:1410:GOL:O3	1.88	0.74
1:B:29:GLN:HE22	1:B:83:VAL:H	1.35	0.74
1:F:4:ASN:ND2	1:F:7:ASP:H	1.86	0.74
1:J:4:ASN:ND2	1:J:7:ASP:H	1.86	0.74
1:M:111:LYS:O	1:M:115:GLU:HG3	1.88	0.74
1:N:29:GLN:HE22	1:N:83:VAL:H	1.33	0.73
1:J:127[B]:ARG:HB3	4:J:1910:GOL:O3	1.88	0.73
1:C:58[B]:ARG:NH2	1:D:168[B]:SER:C	2.42	0.73
1:A:168[A]:SER:CB	1:B:58[A]:ARG:HH22	1.93	0.73
1:B:81:LYS:HE2	3:B:1005:SO4:O1	1.88	0.73
1:G:168[A]:SER:OG	5:G:1608[A]:FEC:HAC2	1.88	0.73
5:M:2207[A]:FEC:HBB2	1:N:168[A]:SER:HB3	1.70	0.73
1:L:75:THR:OG1	1:L:77[B]:GLN:HG3	1.89	0.73
1:O:58[B]:ARG:NH2	1:P:168[B]:SER:HB3	2.01	0.73
1:I:127[B]:ARG:CB	4:I:1810:GOL:O1	2.25	0.72
1:J:29:GLN:HE22	1:J:83:VAL:H	1.35	0.72
1:K:114:LYS:HE2	3:K:1504:SO4:O1	1.90	0.72
1:B:168[B]:SER:OG	5:B:1107[B]:FEC:HAC2	1.90	0.71
1:E:127[A]:ARG:HB3	4:E:1410:GOL:O3	1.90	0.71
1:A:58[B]:ARG:NH2	1:B:168[B]:SER:HB3	2.05	0.71
1:P:4:ASN:ND2	1:P:7:ASP:H	1.88	0.71
1:C:58[B]:ARG:NH2	1:D:168[B]:SER:N	2.38	0.71
1:C:147:LYS:HD2	1:G:5[A]:ARG:NH1	2.05	0.71
1:M:127[B]:ARG:NH2	4:M:2210:GOL:O1	2.23	0.71
1:B:93[B]:GLU:OE2	1:B:147:LYS:NZ	2.23	0.71
1:I:127[B]:ARG:HD2	4:I:1810:GOL:O1	1.91	0.71
1:C:78:LYS:NZ	4:D:1211:GOL:H12	2.06	0.71
1:J:127[A]:ARG:HB3	4:J:1910:GOL:O3	1.90	0.71
1:D:168[B]:SER:CB	5:D:1311[B]:FEC:HBC1	2.21	0.70
5:I:1807[A]:FEC:HHC	5:I:1807[A]:FEC:HBC2	1.72	0.70
1:D:123:ARG:O	1:D:127[B]:ARG:HG2	1.91	0.70
1:G:168[A]:SER:HB2	1:H:58[A]:ARG:CZ	2.15	0.69
1:O:162:SER:N	3:O:2406:SO4:O3	2.25	0.69
1:B:127[A]:ARG:HD2	4:B:1110:GOL:O1	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:168[A]:SER:H	1:N:58[A]:ARG:NH1	1.91	0.69
1:M:169[B]:LYS:NZ	1:N:165:GLY:HA3	2.06	0.69
1:L:29:GLN:HE22	1:L:83:VAL:H	1.40	0.69
1:D:169[B]:LYS:CE	7:D:9732:HOH:O	2.41	0.69
4:M:2211:GOL:H12	1:N:78:LYS:NZ	2.08	0.68
1:E:110:LEU:HD11	1:E:126:GLU:HG3	1.76	0.68
1:G:168[A]:SER:N	1:H:58[A]:ARG:NH2	2.38	0.68
5:L:2108[B]:FEC:HBC2	5:L:2108[B]:FEC:HHC	1.75	0.68
1:M:127[A]:ARG:HD2	4:M:2210:GOL:O1	1.93	0.68
5:M:2207[B]:FEC:HAC2	1:N:168[B]:SER:HB2	1.76	0.68
1:K:168[A]:SER:HB3	5:L:2108[A]:FEC:HBC1	1.76	0.68
1:L:168[B]:SER:HB3	5:L:2108[B]:FEC:HBC1	1.74	0.68
1:O:164:THR:HA	7:O:2485:HOH:O	1.94	0.68
1:D:122:ALA:O	1:D:126:GLU:HG3	1.95	0.67
1:C:58[B]:ARG:NH2	1:D:168[B]:SER:O	2.28	0.66
1:E:110:LEU:HD23	1:E:114:LYS:HD2	1.78	0.66
1:D:4:ASN:HD22	1:D:7:ASP:HB2	1.60	0.66
1:O:31:MET:HG3	5:P:2507[A]:FEC:HBD1	1.76	0.66
1:F:127[A]:ARG:HD3	4:F:1510:GOL:O1	1.96	0.66
1:I:123:ARG:HB3	1:I:127[B]:ARG:NH2	2.11	0.66
1:M:168[A]:SER:OG	5:M:2207[A]:FEC:HAC2	1.96	0.66
1:D:75:THR:OG1	1:D:77[A]:GLN:HG2	1.97	0.65
5:D:1311[B]:FEC:HBC2	5:D:1311[B]:FEC:HHC	1.78	0.65
5:G:1608[A]:FEC:HBC2	5:G:1608[A]:FEC:HHC	1.78	0.65
1:P:168[B]:SER:OG	5:P:2507[B]:FEC:HAC2	1.97	0.65
1:C:162:SER:N	3:C:1206:SO4:O3	2.31	0.64
1:G:156:LYS:HE3	7:G:1708:HOH:O	1.98	0.64
1:A:168[A]:SER:OG	5:B:1107[A]:FEC:HAC2	1.98	0.63
1:I:168[A]:SER:OG	5:I:1807[A]:FEC:HAC2	1.97	0.63
1:C:168[A]:SER:C	1:D:58[A]:ARG:HH22	2.01	0.63
1:I:127[B]:ARG:HB3	4:I:1810:GOL:O1	1.97	0.63
1:K:168[A]:SER:OG	5:L:2108[A]:FEC:HAC2	1.99	0.63
1:D:168[B]:SER:OG	5:D:1311[B]:FEC:HBC1	1.99	0.62
5:B:1107[B]:FEC:HBC1	5:B:1107[B]:FEC:HHC	1.82	0.62
1:E:155:ALA:HA	1:P:149:LEU:HD13	1.81	0.62
1:K:31:MET:HG3	5:L:2108[A]:FEC:HBD1	1.81	0.62
1:O:168[B]:SER:CB	5:P:2507[B]:FEC:O2C	2.46	0.62
1:C:164:THR:O	1:D:169[B]:LYS:HD2	1.99	0.62
1:J:4:ASN:HD22	1:J:7:ASP:H	1.45	0.62
1:P:31:MET:HG3	5:P:2507[B]:FEC:HBD1	1.82	0.62
1:P:110:LEU:HD11	1:P:126:GLU:HG2	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:GLU:OE1	1:C:74:PRO:HD2	1.98	0.62
1:M:58[B]:ARG:HH12	1:N:168[B]:SER:HB3	1.64	0.62
1:L:5:ARG:HG2	3:L:2102:SO4:O1	1.99	0.62
1:L:168[A]:SER:OG	5:L:2108[A]:FEC:O2B	2.18	0.62
4:M:2211:GOL:H12	1:N:78:LYS:HZ3	1.65	0.62
1:A:62:ASN:OD1	4:A:1010:GOL:H12	2.00	0.61
1:B:145:HIS:HE1	1:H:41:ASP:OD2	1.82	0.61
1:O:110:LEU:HD11	1:O:126:GLU:HG3	1.81	0.61
1:E:168[B]:SER:HB3	5:F:1507[B]:FEC:HBB2	1.81	0.61
1:J:110:LEU:CD2	1:J:114:LYS:HE2	2.31	0.61
1:E:169[A]:LYS:O	1:E:169[A]:LYS:HG3	2.00	0.61
1:M:168[A]:SER:C	1:N:58[A]:ARG:NH2	2.54	0.61
1:K:169[B]:LYS:HD2	1:K:169[B]:LYS:N	2.16	0.61
4:K:2011:GOL:O1	1:L:77[A]:GLN:HB3	2.00	0.61
1:O:168[A]:SER:CB	1:P:58[A]:ARG:HH12	2.13	0.61
1:C:169[B]:LYS:HD3	1:C:169[B]:LYS:H	1.66	0.60
1:B:110:LEU:HD21	1:B:114:LYS:HE3	1.83	0.60
1:D:169[B]:LYS:HE3	7:D:9732:HOH:O	2.00	0.59
1:I:110:LEU:CD2	1:I:114:LYS:HD2	2.32	0.59
1:E:127[B]:ARG:HD2	4:E:1410:GOL:O3	2.01	0.59
1:O:168[A]:SER:HB2	1:P:58[A]:ARG:NH1	2.15	0.59
1:P:168[B]:SER:CB	5:P:2507[B]:FEC:HAC2	2.32	0.59
3:P:2501:SO4:O3	7:P:9918:HOH:O	2.17	0.59
1:G:58[B]:ARG:NH1	1:H:168[B]:SER:H	2.01	0.59
1:M:169[B]:LYS:HZ1	1:N:165:GLY:HA3	1.68	0.59
1:P:169[B]:LYS:O	1:P:169[B]:LYS:HG3	2.03	0.59
1:I:108:GLN:HG2	7:I:9786:HOH:O	2.01	0.59
1:E:82:VAL:HG11	1:F:76:THR:HG21	1.85	0.58
1:K:58[B]:ARG:HG3	1:K:58[B]:ARG:HH11	1.67	0.58
1:M:168[A]:SER:HB3	5:M:2207[A]:FEC:HBC1	1.85	0.58
1:D:169[B]:LYS:NZ	7:D:9732:HOH:O	2.36	0.58
1:O:62:ASN:OD1	4:O:2410:GOL:H12	2.03	0.58
5:I:1807[A]:FEC:HBB2	1:J:168[A]:SER:OG	2.03	0.58
1:D:168[B]:SER:HB3	5:D:1311[B]:FEC:HBC1	1.84	0.57
1:J:127[B]:ARG:HD2	4:J:1910:GOL:O3	2.04	0.57
1:A:58[B]:ARG:NH2	1:B:168[B]:SER:CB	2.67	0.57
1:C:168[A]:SER:OG	5:D:1311[A]:FEC:HAC2	2.05	0.57
1:F:168[B]:SER:CB	5:F:1507[B]:FEC:HAC2	2.34	0.57
5:M:2207[B]:FEC:HAC2	1:N:168[B]:SER:CB	2.34	0.57
1:J:88:VAL:HG23	7:J:955:HOH:O	2.03	0.57
1:O:169[B]:LYS:HD2	1:P:164:THR:O	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:168[B]:SER:HA	5:I:1807[B]:FEC:O2C	2.05	0.57
1:C:78:LYS:HZ3	4:D:1211:GOL:H12	1.69	0.57
1:C:82:VAL:HG11	1:D:76:THR:HG21	1.87	0.57
1:C:168[A]:SER:CB	5:D:1311[A]:FEC:HAC2	2.34	0.57
1:C:168[B]:SER:HB3	5:D:1311[B]:FEC:HBB2	1.87	0.57
1:M:58[B]:ARG:NH1	1:N:168[B]:SER:HB3	2.20	0.57
1:O:57:MET:HB3	5:P:2507[B]:FEC:C1D	2.34	0.57
1:B:163:SER:HB2	3:B:1106:SO4:O2	2.05	0.57
1:J:162:SER:N	3:J:1906:SO4:O1	2.37	0.57
1:P:110:LEU:HD11	1:P:126:GLU:CG	2.34	0.57
1:A:5:ARG:HD2	1:A:8:ARG:NH1	2.19	0.56
1:B:57:MET:HB3	5:B:1107[A]:FEC:C1D	2.35	0.56
1:F:145:HIS:HE1	1:L:41:ASP:OD2	1.88	0.56
1:A:110:LEU:CD2	1:A:114:LYS:HE3	2.35	0.56
1:M:54:ILE:HG21	1:N:169[B]:LYS:O	2.04	0.56
1:P:57:MET:HB3	5:P:2507[A]:FEC:C1D	2.36	0.56
1:A:41:ASP:OD2	1:N:145:HIS:HE1	1.89	0.56
1:F:168[B]:SER:HB2	5:F:1507[B]:FEC:HAC2	1.86	0.56
1:M:110:LEU:HD23	1:M:114:LYS:HD2	1.88	0.56
5:P:2507[A]:FEC:HBC2	5:P:2507[A]:FEC:HHC	1.87	0.56
1:K:76:THR:HG21	1:L:82:VAL:HG11	1.87	0.56
1:O:128:ILE:O	1:O:132:GLU:HG2	2.05	0.56
1:O:168[B]:SER:OG	5:P:2507[B]:FEC:O2B	2.24	0.56
1:C:4:ASN:OD1	1:C:7:ASP:HB2	2.06	0.56
1:E:110:LEU:HD11	1:E:126:GLU:CG	2.35	0.56
5:I:1807[A]:FEC:C1D	1:J:57:MET:HB3	2.35	0.55
1:E:41:ASP:OD2	1:P:145:HIS:HE1	1.89	0.55
5:G:1608[A]:FEC:O2C	1:H:168[A]:SER:HB3	2.05	0.55
1:E:114:LYS:NZ	3:E:1304:SO4:O3	2.31	0.55
5:M:2207[A]:FEC:HBC2	5:M:2207[A]:FEC:HHC	1.88	0.55
1:B:147:LYS:HE3	7:B:1149:HOH:O	2.07	0.55
1:M:169[A]:LYS:O	1:N:54:ILE:HG21	2.06	0.55
5:M:2207[A]:FEC:O2C	1:N:168[A]:SER:HB3	2.07	0.55
1:D:57:MET:HB3	5:D:1311[B]:FEC:C1B	2.36	0.55
1:D:127[B]:ARG:HD3	7:D:9685:HOH:O	2.05	0.55
1:M:127[B]:ARG:NE	4:M:2210:GOL:C1	2.70	0.55
1:B:168[B]:SER:CB	5:B:1107[B]:FEC:HAC2	2.37	0.54
1:M:57:MET:HB3	5:M:2207[A]:FEC:C1B	2.37	0.54
1:K:110:LEU:HD11	1:K:126:GLU:CG	2.38	0.54
1:L:144:SER:CB	3:L:2103:SO4:O1	2.55	0.54
1:I:58[B]:ARG:NH2	1:J:168[B]:SER:HB3	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:GLU:CD	1:G:4:ASN:HB2	2.28	0.54
1:A:110:LEU:HD11	1:A:126:GLU:HG2	1.88	0.54
1:E:20:ARG:HH22	5:F:1507[B]:FEC:CGD	2.20	0.54
1:G:110:LEU:HD11	1:G:126:GLU:CG	2.38	0.54
1:I:57:MET:HB3	5:I:1807[A]:FEC:C1B	2.38	0.54
1:P:27:ILE:HD11	1:P:57:MET:HA	1.90	0.54
1:F:57:MET:HB3	5:F:1507[A]:FEC:C1D	2.37	0.54
1:A:110:LEU:HD11	1:A:126:GLU:CG	2.38	0.53
1:C:4:ASN:ND2	1:C:6:GLU:H	2.06	0.53
1:C:155:ALA:O	1:E:156:LYS:HE2	2.08	0.53
1:B:114:LYS:HD3	3:B:1104:SO4:O2	2.08	0.53
1:P:57:MET:HB3	5:P:2507[B]:FEC:C1B	2.39	0.53
1:I:127[A]:ARG:CG	4:I:1810:GOL:O1	2.45	0.53
1:C:57:MET:HB3	5:D:1311[B]:FEC:C1D	2.38	0.53
1:F:110:LEU:HD22	1:F:114:LYS:HE2	1.90	0.53
1:A:168[A]:SER:H	1:B:58[A]:ARG:HH12	1.56	0.53
1:B:110:LEU:HD11	1:B:126:GLU:HG3	1.91	0.53
1:D:88:VAL:HG12	1:D:146:ILE:HD13	1.90	0.53
1:E:158:ALA:HB1	1:P:145:HIS:CD2	2.43	0.53
1:H:88:VAL:HG12	1:H:146:ILE:HD13	1.91	0.53
1:J:114:LYS:NZ	3:J:1904:SO4:O2	2.25	0.53
1:C:78:LYS:HZ1	4:D:1211:GOL:H12	1.72	0.53
1:M:169[B]:LYS:HZ3	1:N:165:GLY:HA3	1.74	0.53
1:I:127[A]:ARG:HD2	7:I:9733:HOH:O	2.08	0.52
1:M:58[B]:ARG:HH12	1:N:168[B]:SER:H	1.56	0.52
1:C:169[A]:LYS:O	1:D:54:ILE:HG21	2.09	0.52
1:D:78:LYS:HZ3	4:D:1211:GOL:C2	2.23	0.52
1:G:168[A]:SER:C	1:H:58[A]:ARG:HH21	2.12	0.52
1:K:110:LEU:HD23	1:K:114:LYS:HD2	1.90	0.52
1:A:54:ILE:HG21	1:B:169[B]:LYS:O	2.08	0.52
1:B:110:LEU:CD2	1:B:114:LYS:HE3	2.40	0.52
1:C:31:MET:HG3	5:D:1311[A]:FEC:HBD1	1.90	0.52
1:F:127[A]:ARG:HB3	4:F:1510:GOL:O1	2.09	0.52
1:K:110:LEU:HD11	1:K:126:GLU:HG3	1.92	0.52
1:K:149:LEU:HD13	1:O:155:ALA:HA	1.90	0.52
1:M:127[B]:ARG:HB3	4:M:2210:GOL:H12	1.92	0.52
1:K:169[A]:LYS:HB2	7:K:9227:HOH:O	2.10	0.52
5:G:1608[B]:FEC:O1C	1:H:168[B]:SER:OG	2.28	0.52
5:P:2507[B]:FEC:HBC1	5:P:2507[B]:FEC:HHC	1.92	0.52
1:M:168[A]:SER:CB	5:M:2207[A]:FEC:HBC1	2.39	0.52
3:A:1105:SO4:O4	1:B:77:GLN:HG2	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168[A]:SER:O	1:D:58[A]:ARG:CZ	2.57	0.52
1:D:164:THR:HA	7:D:9672:HOH:O	2.09	0.52
1:E:58[A]:ARG:HG2	4:E:1410:GOL:O1	2.10	0.52
1:K:93[B]:GLU:OE1	7:K:9178:HOH:O	2.18	0.52
1:A:169[A]:LYS:O	1:B:54:ILE:HG21	2.10	0.52
1:M:163:SER:HB2	3:M:2206:SO4:O4	2.10	0.52
1:P:58[B]:ARG:HG2	4:P:2510:GOL:O3	2.10	0.52
1:D:57:MET:HB3	5:D:1311[A]:FEC:C1D	2.40	0.52
5:G:1608[A]:FEC:O2B	1:H:168[A]:SER:OG	2.27	0.52
5:I:1807[B]:FEC:O1C	1:J:168[B]:SER:OG	2.27	0.52
1:M:127[B]:ARG:HE	4:M:2210:GOL:C1	2.22	0.51
1:D:31:MET:HG3	5:D:1311[B]:FEC:HBD1	1.93	0.51
5:M:2207[B]:FEC:CAC	1:N:168[B]:SER:OG	2.54	0.51
1:A:151:ASP:OD1	1:A:154:LEU:HD12	2.10	0.51
1:E:111:LYS:HG2	1:E:115:GLU:OE2	2.09	0.51
1:M:57:MET:HB3	5:M:2207[B]:FEC:C1D	2.40	0.51
1:N:4:ASN:HD22	1:N:7:ASP:H	1.59	0.51
1:C:89:PRO:CB	1:G:6[A]:GLU:HG3	2.40	0.51
1:E:58[A]:ARG:HG2	4:E:1410:GOL:HO1	1.75	0.51
1:E:168[B]:SER:OG	5:F:1507[B]:FEC:O2B	2.28	0.51
1:G:110:LEU:HD11	1:G:126:GLU:HG3	1.93	0.51
1:A:123:ARG:HB3	1:A:127[B]:ARG:NH2	2.26	0.51
1:E:128:ILE:O	1:E:132:GLU:HG2	2.10	0.51
5:M:2207[A]:FEC:O2B	1:N:168[A]:SER:OG	2.29	0.51
1:K:55:ASP:OD2	1:L:172:VAL:HG13	2.10	0.51
1:O:33:GLN:NE2	1:O:95:ASP:OD2	2.43	0.51
1:B:110:LEU:HD11	1:B:126:GLU:CG	2.40	0.51
1:K:57:MET:HB3	5:L:2108[B]:FEC:C1D	2.41	0.51
1:E:57:MET:HB3	5:F:1507[A]:FEC:C1B	2.41	0.50
1:I:127[B]:ARG:CD	4:I:1810:GOL:HO1	2.23	0.50
1:O:78:LYS:HZ1	4:O:2411:GOL:H12	1.76	0.50
1:G:127[B]:ARG:NE	4:G:1610:GOL:O1	2.44	0.50
1:A:168[A]:SER:OG	5:B:1107[A]:FEC:O1C	2.30	0.50
1:L:31:MET:HG3	5:L:2108[B]:FEC:HBD1	1.94	0.50
1:G:88:VAL:HG12	1:G:146:ILE:HD13	1.94	0.50
1:I:127[B]:ARG:CB	4:I:1810:GOL:HO1	2.25	0.50
1:G:168[A]:SER:HB2	1:H:58[A]:ARG:HH22	0.39	0.50
1:M:110:LEU:HD11	1:M:126:GLU:CG	2.41	0.50
7:A:1167:HOH:O	1:N:145:HIS:HD2	1.94	0.50
1:F:58[B]:ARG:HD3	5:F:1507[B]:FEC:O2B	2.11	0.50
1:O:58[B]:ARG:CZ	1:P:168[B]:SER:H	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:168[A]:SER:HB2	1:J:58[A]:ARG:NH1	2.27	0.50
1:E:168[A]:SER:OG	5:F:1507[A]:FEC:HAC2	2.11	0.49
1:O:110:LEU:HD11	1:O:126:GLU:CG	2.42	0.49
1:C:155:ALA:HA	1:E:149:LEU:HD13	1.94	0.49
1:F:145:HIS:HD2	7:L:2192:HOH:O	1.95	0.49
1:F:156:LYS:HE2	1:L:155:ALA:O	2.12	0.49
1:H:4:ASN:HD22	1:H:7:ASP:HB2	1.77	0.49
1:J:168[B]:SER:OG	1:J:169[B]:LYS:N	2.45	0.49
1:G:168[A]:SER:C	1:H:58[A]:ARG:NH2	2.65	0.49
1:I:65:GLU:HG2	7:J:8968:HOH:O	2.12	0.49
1:I:127[B]:ARG:HD3	4:I:1713:GOL:C3	2.42	0.49
1:C:89:PRO:HB2	1:G:6[A]:GLU:HG3	1.93	0.49
1:B:165:GLY:HA3	7:B:1250:HOH:O	2.12	0.49
1:I:78:LYS:NZ	4:J:1811:GOL:H12	2.27	0.49
1:J:127[B]:ARG:NH2	7:J:8922:HOH:O	2.44	0.49
1:K:58[B]:ARG:HG3	1:K:58[B]:ARG:NH1	2.28	0.49
1:M:127[B]:ARG:HG3	1:M:127[B]:ARG:HH11	1.78	0.49
1:F:4:ASN:HD22	1:F:7:ASP:H	1.59	0.49
1:I:81:LYS:HE3	1:I:82:VAL:N	2.24	0.49
1:K:168[B]:SER:HA	5:L:2108[B]:FEC:CGC	2.34	0.49
1:O:168[B]:SER:HB2	5:P:2507[B]:FEC:HBC2	1.93	0.49
1:I:35:TYR:OH	5:I:1807[B]:FEC:O2A	2.29	0.49
1:D:128:ILE:O	1:D:132:GLU:HG2	2.12	0.48
1:I:88:VAL:HB	1:I:89:PRO:HD3	1.95	0.48
1:K:168[B]:SER:OG	5:L:2108[B]:FEC:O2B	2.30	0.48
1:L:88:VAL:HG12	1:L:146:ILE:HD13	1.95	0.48
1:B:127[A]:ARG:HH22	1:N:130:GLU:CD	2.17	0.48
1:P:79:GLU:HG2	7:P:9558:HOH:O	2.12	0.48
1:E:88:VAL:HG12	1:E:146:ILE:HD13	1.95	0.48
1:I:168[B]:SER:HA	5:I:1807[B]:FEC:CGC	2.43	0.48
1:C:33:GLN:NE2	1:C:95:ASP:OD2	2.44	0.48
1:K:89:PRO:O	1:K:93[B]:GLU:HG3	2.12	0.48
1:O:127[B]:ARG:NE	7:O:2414:HOH:O	2.42	0.48
1:E:62:ASN:ND2	7:E:9906:HOH:O	2.47	0.48
1:C:110:LEU:HD11	1:C:126:GLU:HG2	1.95	0.48
1:F:51:LEU:HD21	1:F:164:THR:HB	1.96	0.48
1:I:40:MET:HE1	7:I:996:HOH:O	2.12	0.48
1:L:169[B]:LYS:NZ	7:L:2166:HOH:O	2.47	0.48
1:M:127[B]:ARG:NH1	7:M:823:HOH:O	2.47	0.48
1:O:52:ILE:O	1:O:56:GLU:HG2	2.13	0.48
1:L:4:ASN:ND2	1:L:7:ASP:H	2.11	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168[A]:SER:N	1:B:58[A]:ARG:NH2	2.60	0.48
1:D:132:GLU:OE1	1:D:132:GLU:HA	2.14	0.48
1:G:57:MET:HB3	5:G:1608[B]:FEC:C1D	2.43	0.48
1:I:127[B]:ARG:HE	1:I:127[B]:ARG:HB2	1.37	0.48
1:F:128:ILE:O	1:F:132:GLU:HG2	2.14	0.47
1:I:57:MET:HB3	5:I:1807[B]:FEC:C1D	2.44	0.47
1:I:81:LYS:HD2	1:I:81:LYS:HA	1.44	0.47
1:M:169[A]:LYS:O	1:M:169[A]:LYS:HG3	2.13	0.47
1:A:57:MET:HB3	5:B:1107[A]:FEC:C1B	2.44	0.47
1:C:57:MET:HB3	5:D:1311[A]:FEC:C1B	2.44	0.47
1:M:14:GLU:O	1:M:14:GLU:HG2	2.14	0.47
1:O:58[B]:ARG:NH2	1:P:168[B]:SER:C	2.65	0.47
1:M:169[B]:LYS:HB2	1:M:169[B]:LYS:HE3	1.64	0.47
1:A:127[B]:ARG:NE	7:A:1195:HOH:O	2.47	0.47
1:C:13:ILE:HD13	1:C:72:GLY:HA3	1.95	0.47
5:F:1507[B]:FEC:HHC	5:F:1507[B]:FEC:CBC	2.44	0.47
1:P:133:GLN:NE2	7:P:676:HOH:O	2.47	0.47
1:L:88:VAL:HB	1:L:89:PRO:HD3	1.97	0.47
5:M:2207[B]:FEC:HHC	5:M:2207[B]:FEC:HBC2	1.96	0.47
1:A:168[A]:SER:HB2	1:B:58[A]:ARG:HH22	1.75	0.47
1:K:168[B]:SER:HB2	5:L:2108[B]:FEC:O2C	2.12	0.47
5:P:2507[B]:FEC:HHC	5:P:2507[B]:FEC:CBC	2.45	0.47
1:B:147:LYS:HE2	7:B:1230:HOH:O	2.14	0.47
1:F:58[B]:ARG:HH11	5:F:1507[B]:FEC:HBB2	1.80	0.47
5:G:1608[B]:FEC:HBC1	1:H:168[B]:SER:OG	2.15	0.47
1:J:161:PRO:CA	3:J:1906:SO4:O1	2.54	0.47
1:G:33:GLN:NE2	1:G:95:ASP:OD2	2.46	0.47
1:I:168[A]:SER:HB3	5:I:1807[A]:FEC:HBC1	1.97	0.47
1:P:31:MET:HG3	5:P:2507[A]:FEC:HBA2	1.97	0.47
1:D:127[B]:ARG:NH1	7:D:9685:HOH:O	2.48	0.47
1:D:168[B]:SER:HG	5:D:1311[B]:FEC:CGC	2.10	0.47
5:I:1807[B]:FEC:HBD1	1:J:31:MET:HG3	1.97	0.47
1:N:4:ASN:ND2	1:N:7:ASP:H	2.13	0.47
1:C:147:LYS:HD2	1:G:5[A]:ARG:HH12	1.79	0.46
1:M:65:GLU:O	1:M:69:GLU:HG3	2.15	0.46
1:A:127[B]:ARG:NH2	7:A:1195:HOH:O	2.48	0.46
1:C:31:MET:HG3	5:D:1311[B]:FEC:HBA2	1.97	0.46
1:D:88:VAL:CG1	1:D:146:ILE:HD13	2.46	0.46
1:D:111:LYS:HD2	7:D:526:HOH:O	2.15	0.46
1:E:33:GLN:NE2	1:E:95:ASP:OD2	2.48	0.46
1:H:29:GLN:NE2	1:H:83:VAL:H	2.00	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:127[B]:ARG:HG2	4:I:1810:GOL:C1	2.45	0.46
1:E:169[A]:LYS:O	1:F:54:ILE:HG21	2.14	0.46
1:F:4:ASN:HB2	3:F:1502:SO4:O2	2.15	0.46
1:I:123:ARG:HB3	1:I:127[B]:ARG:HH22	1.81	0.46
1:A:88:VAL:HG12	1:A:146:ILE:HD13	1.97	0.46
1:E:11:LYS:NZ	7:E:713:HOH:O	2.49	0.46
1:G:88:VAL:HB	1:G:89:PRO:HD3	1.97	0.46
1:M:58[B]:ARG:NH1	1:N:168[B]:SER:H	2.12	0.46
1:G:77:GLN:HB3	4:G:1611:GOL:O1	2.15	0.46
1:F:127[A]:ARG:NH1	1:P:130:GLU:OE2	2.48	0.46
1:H:45:LEU:HG	1:H:157:ILE:HG21	1.97	0.46
1:H:62:ASN:ND2	4:H:1710:GOL:O3	2.49	0.46
1:O:169[B]:LYS:O	1:P:54:ILE:HG21	2.15	0.46
1:O:142:ILE:HG22	1:O:146:ILE:HD12	1.98	0.46
1:G:168[A]:SER:O	1:H:58[A]:ARG:NH2	2.48	0.46
5:M:2207[A]:FEC:CGC	1:N:168[A]:SER:HA	2.46	0.46
5:I:1807[A]:FEC:CMD	1:J:61:GLU:HB2	2.46	0.46
1:M:168[A]:SER:O	1:N:58[A]:ARG:NH2	2.49	0.46
1:B:27:ILE:HD11	1:B:57:MET:HA	1.97	0.45
1:B:127[A]:ARG:HD2	4:B:1110:GOL:HO1	1.77	0.45
1:E:58[B]:ARG:NH2	1:F:168[B]:SER:O	2.47	0.45
1:F:123:ARG:NH1	1:F:126:GLU:OE2	2.50	0.45
1:L:68:LYS:HD3	1:L:74:PRO:HD3	1.98	0.45
1:F:127[B]:ARG:HB3	4:F:1510:GOL:O1	2.17	0.45
1:O:108[A]:GLN:NE2	7:O:2478:HOH:O	2.49	0.45
1:C:88:VAL:HG12	1:C:146:ILE:HD13	1.99	0.45
1:D:133:GLN:NE2	7:D:499:HOH:O	2.49	0.45
5:I:1807[B]:FEC:HHC	5:I:1807[B]:FEC:CBC	2.47	0.45
1:L:4:ASN:HD22	1:L:7:ASP:H	1.64	0.45
1:L:61:GLU:O	1:L:65:GLU:HG3	2.16	0.45
1:M:127[B]:ARG:HG3	1:M:127[B]:ARG:NH1	2.30	0.45
1:P:58[A]:ARG:NH2	7:P:9899:HOH:O	2.49	0.45
1:P:61:GLU:HB2	5:P:2507[A]:FEC:CMD	2.47	0.45
1:A:57:MET:HB3	5:B:1107[B]:FEC:C1D	2.46	0.45
1:G:104:GLU:OE2	1:N:8[B]:ARG:NH2	2.49	0.45
1:I:110:LEU:HD11	1:I:126:GLU:CG	2.46	0.45
1:N:111:LYS:O	1:N:115:GLU:HG3	2.17	0.45
1:A:82:VAL:HG11	1:B:76:THR:HG21	1.99	0.45
1:A:169[A]:LYS:HD2	7:B:1250:HOH:O	2.17	0.45
1:F:61:GLU:HB2	5:F:1507[A]:FEC:CMD	2.46	0.45
1:L:127[B]:ARG:NH2	7:L:2109:HOH:O	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:58[B]:ARG:NH2	1:P:168[B]:SER:O	2.49	0.45
1:A:4:ASN:ND2	7:A:1208:HOH:O	2.49	0.45
1:F:112:VAL:O	1:F:116:GLN:HG2	2.16	0.45
1:I:147:LYS:NZ	3:I:1803:SO4:O3	2.50	0.45
1:M:58[B]:ARG:NH2	1:N:168[B]:SER:CB	2.78	0.45
1:I:110:LEU:HD11	1:I:126:GLU:HG2	1.98	0.45
1:P:168[B]:SER:OG	5:P:2507[B]:FEC:O1C	2.29	0.45
1:M:76:THR:HG21	1:N:82:VAL:HG11	1.99	0.45
1:N:133:GLN:NE2	7:N:2315:HOH:O	2.50	0.45
1:O:43:GLY:HA2	1:O:162:SER:HB3	1.99	0.45
1:P:127[B]:ARG:NE	4:P:2510:GOL:O1	2.50	0.45
1:M:161:PRO:HB3	3:M:2206:SO4:O2	2.17	0.45
1:C:168[B]:SER:OG	5:D:1311[B]:FEC:O2B	2.35	0.44
1:G:151:ASP:HB2	7:G:1676:HOH:O	2.17	0.44
1:B:61:GLU:HB2	5:B:1107[A]:FEC:CMD	2.47	0.44
1:F:58[B]:ARG:HH11	5:F:1507[B]:FEC:CBB	2.30	0.44
1:J:33:GLN:OE1	1:J:95:ASP:OD2	2.35	0.44
1:J:110:LEU:HD11	1:J:126:GLU:CG	2.38	0.44
1:L:57:MET:HB3	5:L:2108[A]:FEC:C1D	2.47	0.44
1:L:150:GLY:HA3	3:L:2107:SO4:O2	2.16	0.44
1:M:127[B]:ARG:NH2	7:M:823:HOH:O	2.49	0.44
1:O:127[B]:ARG:HG3	1:O:127[B]:ARG:HH11	1.83	0.44
1:A:122:ALA:O	1:A:126:GLU:HG3	2.18	0.44
1:A:168[B]:SER:HB2	5:B:1107[B]:FEC:HBC2	1.31	0.44
1:F:152:THR:CG2	1:L:152:THR:HA	2.48	0.44
1:H:160:THR:HB	1:H:161:PRO:HD2	1.99	0.44
1:I:112:VAL:O	1:I:116:GLN:HG2	2.18	0.44
1:B:57:MET:HB3	5:B:1107[B]:FEC:C1B	2.48	0.44
1:D:168[A]:SER:OG	5:D:1311[A]:FEC:HBB2	2.18	0.44
1:F:5:ARG:HD2	1:F:8:ARG:NH1	2.33	0.44
1:G:82:VAL:HG11	1:H:76:THR:HG21	1.99	0.44
1:L:127[A]:ARG:HD2	7:L:2162:HOH:O	2.18	0.44
1:D:169[B]:LYS:HG2	7:D:9732:HOH:O	2.18	0.44
1:E:6:GLU:OE2	1:E:9:LYS:HD2	2.17	0.44
1:I:29:GLN:O	1:I:33:GLN:HG3	2.17	0.44
1:M:110:LEU:HD11	1:M:126:GLU:HG2	1.99	0.44
5:M:2207[A]:FEC:HMD2	1:N:61:GLU:HB2	1.99	0.44
1:O:76:THR:HG21	1:P:82:VAL:HG11	2.00	0.44
1:A:78:LYS:HE2	3:A:1105:SO4:S	2.55	0.44
1:L:168[B]:SER:OG	5:L:2108[B]:FEC:HMC1	2.18	0.44
1:B:169[B]:LYS:O	1:B:169[B]:LYS:HG3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127[A]:ARG:HD3	4:E:1410:GOL:O3	2.18	0.44
5:I:1807[A]:FEC:O1C	1:J:168[A]:SER:HA	2.16	0.44
1:K:82:VAL:HG11	1:L:76:THR:HG21	2.00	0.44
1:L:105:ALA:O	1:L:108:GLN:HB2	2.18	0.44
1:P:4:ASN:HD22	1:P:7:ASP:H	1.60	0.43
1:B:127[B]:ARG:HB3	4:B:1110:GOL:O1	2.17	0.43
1:I:54:ILE:HG21	1:J:169[B]:LYS:O	2.19	0.43
1:A:7:ASP:OD1	1:O:4:ASN:ND2	2.51	0.43
1:D:33:GLN:OE1	1:D:95:ASP:OD2	2.35	0.43
1:D:127[A]:ARG:HD2	6:D:1310:3PY:O1	2.17	0.43
1:M:110:LEU:HD11	1:M:126:GLU:HG3	2.00	0.43
1:I:82:VAL:HG11	1:J:76:THR:HG21	2.00	0.43
1:O:127[B]:ARG:NH2	7:O:2437:HOH:O	2.51	0.43
1:C:110:LEU:HD11	1:C:126:GLU:CG	2.48	0.43
1:M:78:LYS:HE2	4:M:2211:GOL:O2	2.18	0.43
1:A:110:LEU:HD21	1:A:114:LYS:HE3	1.98	0.43
1:C:41:ASP:HB3	1:E:145:HIS:CE1	2.54	0.43
1:C:122:ALA:O	1:C:126:GLU:HG3	2.19	0.43
1:H:12:VAL:HG11	1:H:118:ASP:OD2	2.19	0.43
1:M:13:ILE:HD13	1:M:72:GLY:HA3	2.00	0.43
1:P:142:ILE:O	1:P:146:ILE:HG12	2.19	0.43
1:P:161:PRO:HA	3:P:2506:SO4:O4	2.18	0.43
1:C:123:ARG:NH2	1:C:126:GLU:OE2	2.49	0.43
1:D:110:LEU:O	1:D:114:LYS:HG3	2.18	0.43
1:G:155:ALA:O	1:I:156:LYS:HD3	2.19	0.43
1:D:78:LYS:NZ	4:D:1211:GOL:O2	2.49	0.43
1:F:58[B]:ARG:NH1	5:F:1507[B]:FEC:HBB2	2.34	0.43
1:G:110:LEU:HD11	1:G:126:GLU:HG2	2.00	0.43
1:O:78:LYS:HZ1	4:O:2411:GOL:C1	2.31	0.43
1:O:127[B]:ARG:NH2	7:O:2414:HOH:O	2.50	0.43
1:E:76:THR:HG21	1:F:82:VAL:HG11	2.01	0.43
1:O:61:GLU:HB2	5:P:2507[B]:FEC:CMD	2.48	0.43
1:D:43:GLY:HA2	1:D:162:SER:HB3	2.00	0.43
1:K:110:LEU:HD11	1:K:126:GLU:HG2	2.01	0.43
1:L:77[B]:GLN:NE2	7:L:2203:HOH:O	2.52	0.43
1:B:93[A]:GLU:HG2	1:B:94:SER:N	2.33	0.42
5:I:1807[B]:FEC:HHC	5:I:1807[B]:FEC:HBC2	2.01	0.42
1:N:27:ILE:HD11	1:N:57:MET:HA	2.00	0.42
1:F:58[B]:ARG:HG2	5:F:1507[B]:FEC:HBB1	2.01	0.42
1:G:161:PRO:HA	3:G:1606:SO4:O3	2.19	0.42
1:K:78:LYS:NZ	7:K:9116:HOH:O	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:1507[B]:FEC:HHC	5:F:1507[B]:FEC:HBC1	2.00	0.42
5:G:1608[A]:FEC:C1D	1:H:57:MET:HB3	2.48	0.42
1:A:34:HIS:HE1	7:A:1152:HOH:O	2.02	0.42
1:C:68:LYS:HD2	1:C:68:LYS:HA	1.86	0.42
1:P:128:ILE:O	1:P:132:GLU:HG2	2.19	0.42
5:G:1608[B]:FEC:HAC2	1:H:168[B]:SER:CB	2.49	0.42
1:B:123:ARG:HD3	1:N:126:GLU:OE2	2.19	0.42
1:B:127[A]:ARG:NH2	1:N:130:GLU:OE1	2.53	0.42
1:C:168[B]:SER:HA	5:D:1311[B]:FEC:O2C	2.19	0.42
1:G:127[B]:ARG:NH2	7:G:1638:HOH:O	2.49	0.42
1:H:5:ARG:HD2	1:H:8:ARG:NH1	2.35	0.42
1:M:68:LYS:HA	1:M:68:LYS:HD2	1.89	0.42
1:N:62:ASN:ND2	4:N:2310:GOL:O1	2.52	0.42
1:N:169[B]:LYS:O	1:N:169[B]:LYS:HG3	2.18	0.42
1:C:52:ILE:O	1:C:55:ASP:HB2	2.19	0.42
1:E:58[A]:ARG:HH22	1:F:172:VAL:HG22	1.85	0.42
1:H:58[A]:ARG:NH1	1:H:58[A]:ARG:HG3	2.35	0.42
5:I:1807[B]:FEC:HAC2	1:J:168[B]:SER:CB	2.49	0.42
1:K:57:MET:HB3	5:L:2108[A]:FEC:C1B	2.50	0.42
1:D:61:GLU:HB2	5:D:1311[A]:FEC:CMD	2.49	0.42
1:I:81:LYS:CE	1:I:82:VAL:H	2.26	0.42
1:J:110:LEU:HD23	1:J:114:LYS:HE2	2.02	0.42
5:P:2507[A]:FEC:HHC	5:P:2507[A]:FEC:CBC	2.50	0.42
1:A:155:ALA:HA	1:N:149:LEU:HD13	2.02	0.41
1:A:168[A]:SER:HB3	5:B:1107[A]:FEC:HBC1	2.00	0.41
1:B:9:LYS:HA	7:B:1142:HOH:O	2.20	0.41
1:E:58[B]:ARG:NH2	1:F:168[B]:SER:N	2.68	0.41
1:G:57:MET:HB3	5:G:1608[A]:FEC:C1B	2.49	0.41
1:L:61:GLU:HB2	5:L:2108[A]:FEC:HMD2	2.02	0.41
1:A:31:MET:HG3	5:B:1107[A]:FEC:HBD1	2.02	0.41
1:B:61:GLU:HB2	5:B:1107[A]:FEC:HMD2	2.02	0.41
1:D:4:ASN:ND2	1:D:7:ASP:H	2.18	0.41
5:G:1608[B]:FEC:C1B	1:H:57:MET:HB3	2.51	0.41
1:A:58[B]:ARG:NH1	1:B:168[B]:SER:H	2.18	0.41
1:A:123:ARG:NH1	1:A:127[B]:ARG:NH1	2.69	0.41
1:P:78:LYS:NZ	7:P:9538:HOH:O	2.53	0.41
1:I:127[A]:ARG:CB	4:I:1810:GOL:HO1	2.24	0.41
1:K:110:LEU:CD2	1:K:114:LYS:HD2	2.49	0.41
1:M:61:GLU:HB2	5:M:2207[B]:FEC:CMD	2.50	0.41
1:P:147:LYS:HA	1:P:147:LYS:HD3	1.85	0.41
1:B:168[A]:SER:OG	5:B:1107[A]:FEC:HBB2	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:GLN:HA	1:D:82:VAL:HG13	2.03	0.41
1:F:57:MET:HB3	5:F:1507[B]:FEC:C1B	2.50	0.41
1:J:58[B]:ARG:NE	4:J:1910:GOL:O1	2.48	0.41
1:A:112:VAL:O	1:A:116:GLN:HG2	2.21	0.41
1:G:104:GLU:OE1	1:N:8[A]:ARG:NH2	2.53	0.41
1:I:58[B]:ARG:NH2	1:J:168[B]:SER:N	2.68	0.41
1:O:57:MET:HB3	5:P:2507[A]:FEC:C1B	2.50	0.41
1:P:52:ILE:O	1:P:56:GLU:HG2	2.21	0.41
1:P:68:LYS:HD2	1:P:68:LYS:HA	1.89	0.41
1:C:65:GLU:O	1:C:69:GLU:HG3	2.21	0.41
1:G:58[A]:ARG:NE	4:G:1610:GOL:O3	2.48	0.41
5:G:1608[A]:FEC:HBC2	5:G:1608[A]:FEC:CHC	2.49	0.41
1:K:110:LEU:HD13	1:P:119:ILE:HG13	2.02	0.41
1:M:58[B]:ARG:NH2	1:N:168[B]:SER:N	2.64	0.41
1:A:168[B]:SER:OG	5:B:1107[B]:FEC:O2B	2.39	0.41
1:D:29:GLN:HE22	1:D:83:VAL:N	2.01	0.41
1:I:5:ARG:HG2	3:I:1802:SO4:O4	2.20	0.41
1:I:127[B]:ARG:NH2	7:I:9733:HOH:O	2.54	0.41
1:M:58[B]:ARG:HH12	1:N:168[B]:SER:CB	2.32	0.41
1:O:127[B]:ARG:NE	4:O:2410:GOL:O3	2.50	0.41
1:A:16:LEU:HD21	1:A:121:THR:HG23	2.02	0.41
1:N:68:LYS:HD2	1:N:68:LYS:HA	1.84	0.41
1:N:112:VAL:O	1:N:116:GLN:HG2	2.21	0.41
1:A:4:ASN:O	1:A:7:ASP:HB3	2.21	0.40
1:A:6:GLU:HB2	7:A:1208:HOH:O	2.20	0.40
1:D:68:LYS:HD2	1:D:68:LYS:HA	1.91	0.40
5:G:1608[A]:FEC:HBA2	5:G:1608[A]:FEC:HHB	2.03	0.40
1:I:31:MET:HG3	5:I:1807[A]:FEC:HBD1	2.03	0.40
1:K:112:VAL:O	1:K:116:GLN:HG2	2.22	0.40
1:F:27:ILE:HD11	1:F:57:MET:HA	2.03	0.40
1:J:160:THR:HB	1:J:161:PRO:HD2	2.03	0.40
1:A:7:ASP:CG	1:O:4:ASN:HD21	2.23	0.40
1:B:52:ILE:O	1:B:56:GLU:HG2	2.22	0.40
1:C:73:GLU:HA	1:C:74:PRO:HD3	1.97	0.40
1:D:29:GLN:NE2	1:D:83:VAL:H	2.02	0.40
1:H:128:ILE:O	1:H:132:GLU:HG2	2.22	0.40
1:K:168[B]:SER:HB3	5:L:2108[B]:FEC:O2C	2.11	0.40
1:L:75:THR:HG1	1:L:77[B]:GLN:HG3	1.86	0.40
1:M:58[B]:ARG:NH2	1:N:168[B]:SER:HB3	2.37	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1802:SO4:S	3:L:2102:SO4:S[9_465]	0.16	2.04
3:I:1802:SO4:O1	3:L:2102:SO4:O3[9_465]	0.22	1.98
3:I:1802:SO4:O4	3:L:2102:SO4:O2[9_465]	0.35	1.85
3:I:1802:SO4:O2	3:L:2102:SO4:O4[9_465]	0.37	1.83
3:I:1802:SO4:O3	3:L:2102:SO4:O1[9_465]	0.49	1.71
3:I:1802:SO4:O3	3:L:2102:SO4:O2[9_465]	2.14	0.06
3:I:1802:SO4:O2	3:L:2102:SO4:O1[9_465]	2.18	0.02

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	171/179 (96%)	170 (99%)	1 (1%)	0	100 100
1	B	173/179 (97%)	170 (98%)	3 (2%)	0	100 100
1	C	172/179 (96%)	169 (98%)	3 (2%)	0	100 100
1	D	174/179 (97%)	173 (99%)	1 (1%)	0	100 100
1	E	173/179 (97%)	170 (98%)	3 (2%)	0	100 100
1	F	172/179 (96%)	170 (99%)	2 (1%)	0	100 100
1	G	173/179 (97%)	171 (99%)	2 (1%)	0	100 100
1	H	173/179 (97%)	171 (99%)	0	2 (1%)	13 4
1	I	173/179 (97%)	168 (97%)	5 (3%)	0	100 100
1	J	172/179 (96%)	169 (98%)	1 (1%)	2 (1%)	13 4
1	K	173/179 (97%)	169 (98%)	4 (2%)	0	100 100
1	L	173/179 (97%)	168 (97%)	5 (3%)	0	100 100
1	M	172/179 (96%)	170 (99%)	2 (1%)	0	100 100
1	N	172/179 (96%)	169 (98%)	1 (1%)	2 (1%)	13 4
1	O	172/179 (96%)	170 (99%)	2 (1%)	0	100 100
1	P	173/179 (97%)	168 (97%)	3 (2%)	2 (1%)	13 4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2761/2864 (96%)	2715 (98%)	38 (1%)	8 (0%)	51 30

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	169[A]	LYS
1	H	169[B]	LYS
1	J	168[A]	SER
1	J	168[B]	SER
1	N	169[A]	LYS
1	N	169[B]	LYS
1	P	169[A]	LYS
1	P	169[B]	LYS

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	143/145 (99%)	140 (98%)	3 (2%)	53 46
1	B	144/145 (99%)	138 (96%)	6 (4%)	30 17
1	C	142/145 (98%)	130 (92%)	12 (8%)	10 3
1	D	145/145 (100%)	138 (95%)	7 (5%)	25 12
1	E	144/145 (99%)	143 (99%)	1 (1%)	84 82
1	F	143/145 (99%)	137 (96%)	6 (4%)	30 17
1	G	145/145 (100%)	144 (99%)	1 (1%)	84 82
1	H	143/145 (99%)	136 (95%)	7 (5%)	25 12
1	I	145/145 (100%)	141 (97%)	4 (3%)	43 33
1	J	143/145 (99%)	137 (96%)	6 (4%)	30 17
1	K	144/145 (99%)	140 (97%)	4 (3%)	43 33
1	L	144/145 (99%)	139 (96%)	5 (4%)	36 24
1	M	144/145 (99%)	143 (99%)	1 (1%)	84 82

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	N	143/145 (99%)	139 (97%)	4 (3%)	43 33
1	O	143/145 (99%)	142 (99%)	1 (1%)	84 82
1	P	145/145 (100%)	140 (97%)	5 (3%)	37 25
All	All	2300/2320 (99%)	2227 (97%)	73 (3%)	44 27

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	78	LYS
1	A	144	SER
1	B	81	LYS
1	B	93[A]	GLU
1	B	93[B]	GLU
1	B	104	GLU
1	B	147	LYS
1	B	166	THR
1	C	4	ASN
1	C	7	ASP
1	C	77	GLN
1	C	111	LYS
1	C	114	LYS
1	C	152[A]	THR
1	C	152[B]	THR
1	C	163	SER
1	C	168[A]	SER
1	C	168[B]	SER
1	C	169[A]	LYS
1	C	169[B]	LYS
1	D	4	ASN
1	D	7	ASP
1	D	77[A]	GLN
1	D	77[B]	GLN
1	D	81	LYS
1	D	169[A]	LYS
1	D	169[B]	LYS
1	E	147	LYS
1	F	4	ASN
1	F	77	GLN
1	F	81	LYS
1	F	111	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	147	LYS
1	F	156	LYS
1	G	108	GLN
1	H	4	ASN
1	H	11	LYS
1	H	58[A]	ARG
1	H	58[B]	ARG
1	H	81	LYS
1	H	110	LEU
1	H	111	LYS
1	I	4	ASN
1	I	77	GLN
1	I	81	LYS
1	I	147	LYS
1	J	4	ASN
1	J	81	LYS
1	J	146	ILE
1	J	152	THR
1	J	169[A]	LYS
1	J	169[B]	LYS
1	K	7	ASP
1	K	77	GLN
1	K	169[A]	LYS
1	K	169[B]	LYS
1	L	4	ASN
1	L	77[A]	GLN
1	L	77[B]	GLN
1	L	81	LYS
1	L	110	LEU
1	M	7	ASP
1	N	4	ASN
1	N	58[A]	ARG
1	N	58[B]	ARG
1	N	77	GLN
1	O	163	SER
1	P	4	ASN
1	P	6	GLU
1	P	93[A]	GLU
1	P	93[B]	GLU
1	P	144	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	B	4	ASN
1	B	29	GLN
1	B	62	ASN
1	B	133	GLN
1	B	145	HIS
1	C	32	ASN
1	C	33	GLN
1	D	4	ASN
1	D	29	GLN
1	D	62	ASN
1	E	32	ASN
1	E	33	GLN
1	F	4	ASN
1	F	29	GLN
1	F	62	ASN
1	F	133	GLN
1	F	145	HIS
1	G	4	ASN
1	G	32	ASN
1	G	33	GLN
1	H	4	ASN
1	H	29	GLN
1	H	62	ASN
1	H	133	GLN
1	I	32	ASN
1	I	33	GLN
1	J	4	ASN
1	J	29	GLN
1	J	62	ASN
1	J	133	GLN
1	K	32	ASN
1	K	33	GLN
1	K	77	GLN
1	L	4	ASN
1	L	29	GLN
1	L	148	ASN
1	M	4	ASN
1	M	32	ASN
1	M	33	GLN
1	N	4	ASN
1	N	29	GLN
1	N	62	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	133	GLN
1	N	145	HIS
1	N	148	ASN
1	O	32	ASN
1	O	33	GLN
1	P	4	ASN
1	P	29	GLN
1	P	62	ASN
1	P	98	GLN
1	P	133	GLN
1	P	145	HIS
1	P	148	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 124 ligands modelled in this entry, 32 are monoatomic - leaving 92 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	SO4	H	1706	-	4,4,4	0.46	0	6,6,6	0.87	0
4	GOL	K	2011	-	5,5,5	4.44	5 (100%)	5,5,5	4.81	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	P	2506	-	4,4,4	0.46	0	6,6,6	0.56	0
4	GOL	G	1611	-	5,5,5	4.39	5 (100%)	5,5,5	4.39	3 (60%)
3	SO4	P	2501	-	4,4,4	1.91	1 (25%)	6,6,6	0.91	0
3	SO4	G	1603	-	4,4,4	2.02	1 (25%)	6,6,6	0.89	0
4	GOL	I	1810	1	5,5,5	4.38	5 (100%)	5,5,5	3.88	3 (60%)
3	SO4	I	1806	-	4,4,4	0.39	0	6,6,6	0.60	0
4	GOL	E	1411	-	5,5,5	4.45	5 (100%)	5,5,5	4.19	3 (60%)
4	GOL	F	1512	-	5,5,5	4.54	5 (100%)	5,5,5	3.72	3 (60%)
3	SO4	M	2206	-	4,4,4	0.23	0	6,6,6	0.40	0
3	SO4	A	1004	-	4,4,4	1.88	1 (25%)	6,6,6	0.92	0
3	SO4	A	1008	-	4,4,4	0.53	0	6,6,6	2.46	2 (33%)
5	FEC	I	1807[B]	1	40,56,56	1.21	4 (10%)	42,90,90	2.03	12 (28%)
3	SO4	L	2102	3	4,4,4	1.95	1 (25%)	6,6,6	0.86	0
4	GOL	J	1811	-	5,5,5	4.52	5 (100%)	5,5,5	5.39	3 (60%)
5	FEC	L	2108[B]	1	40,56,56	1.26	4 (10%)	42,90,90	1.78	9 (21%)
3	SO4	K	2001	-	4,4,4	1.93	1 (25%)	6,6,6	0.95	0
5	FEC	P	2507[A]	1	40,56,56	1.21	4 (10%)	42,90,90	1.97	12 (28%)
3	SO4	K	1504	-	4,4,4	1.94	1 (25%)	6,6,6	0.86	0
4	GOL	B	1110	-	5,5,5	4.51	5 (100%)	5,5,5	4.49	3 (60%)
4	GOL	M	2211	-	5,5,5	4.52	5 (100%)	5,5,5	4.58	3 (60%)
4	GOL	P	2510	-	5,5,5	4.46	5 (100%)	5,5,5	4.69	3 (60%)
5	FEC	D	1311[A]	1	40,56,56	1.25	4 (10%)	42,90,90	2.01	13 (30%)
5	FEC	M	2207[B]	1	40,56,56	1.28	4 (10%)	42,90,90	1.69	14 (33%)
3	SO4	B	1005	-	4,4,4	0.53	0	6,6,6	2.46	2 (33%)
4	GOL	D	1211	-	5,5,5	4.50	5 (100%)	5,5,5	4.66	3 (60%)
4	GOL	I	1713	-	5,5,5	4.48	5 (100%)	5,5,5	5.59	3 (60%)
3	SO4	B	1106	-	4,4,4	0.13	0	6,6,6	1.50	0
4	GOL	M	2210	1	5,5,5	4.51	5 (100%)	5,5,5	4.39	2 (40%)
4	GOL	H	1710	-	5,5,5	4.53	5 (100%)	5,5,5	5.65	3 (60%)
3	SO4	L	2107	-	4,4,4	1.94	1 (25%)	6,6,6	0.86	0
3	SO4	O	2406	-	4,4,4	0.30	0	6,6,6	1.07	0
4	GOL	E	1410	-	5,5,5	4.53	5 (100%)	5,5,5	4.34	3 (60%)
3	SO4	D	1303	-	4,4,4	0.17	0	6,6,6	0.60	0
4	GOL	J	1910	-	5,5,5	4.56	5 (100%)	5,5,5	4.88	3 (60%)
5	FEC	L	2108[A]	1	40,56,56	1.25	3 (7%)	42,90,90	1.84	11 (26%)
4	GOL	O	2411	-	5,5,5	4.42	5 (100%)	5,5,5	3.91	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	F	1502	-	4,4,4	1.91	1 (25%)	6,6,6	0.92	0
5	FEC	F	1507[B]	1	40,56,56	1.25	4 (10%)	42,90,90	1.91	10 (23%)
3	SO4	A	1105	-	4,4,4	0.53	0	6,6,6	2.46	2 (33%)
3	SO4	C	1201	-	4,4,4	1.93	1 (25%)	6,6,6	0.93	0
3	SO4	H	1703	-	4,4,4	0.28	0	6,6,6	0.58	0
6	3PY	D	1310	1	5,5,6	12.83	5 (100%)	5,5,7	7.82	5 (100%)
3	SO4	N	2303	-	4,4,4	0.18	0	6,6,6	0.81	0
3	SO4	F	1501	-	4,4,4	2.02	1 (25%)	6,6,6	0.84	0
3	SO4	N	2306	-	4,4,4	0.18	0	6,6,6	0.76	0
3	SO4	B	1104	-	4,4,4	2.02	1 (25%)	6,6,6	0.89	0
3	SO4	D	1301	-	4,4,4	1.99	1 (25%)	6,6,6	0.88	0
3	SO4	O	2409	-	4,4,4	0.46	0	6,6,6	0.56	0
3	SO4	P	2503	-	4,4,4	0.20	0	6,6,6	0.92	0
3	SO4	F	1506	-	4,4,4	0.26	0	6,6,6	1.31	1 (16%)
3	SO4	A	1001	-	4,4,4	1.80	1 (25%)	6,6,6	0.94	0
3	SO4	I	1801	-	4,4,4	1.93	1 (25%)	6,6,6	0.92	0
3	SO4	L	2101	-	4,4,4	1.91	1 (25%)	6,6,6	0.92	0
5	FEC	G	1608[B]	1	40,56,56	1.23	4 (10%)	42,90,90	1.92	14 (33%)
4	GOL	F	1510	-	5,5,5	4.45	5 (100%)	5,5,5	4.78	3 (60%)
3	SO4	C	1206	-	4,4,4	0.34	0	6,6,6	0.63	0
3	SO4	B	1101	-	4,4,4	1.88	1 (25%)	6,6,6	0.92	0
3	SO4	J	1904	-	4,4,4	1.93	1 (25%)	6,6,6	0.91	0
5	FEC	F	1507[A]	1	40,56,56	1.28	4 (10%)	42,90,90	1.69	13 (30%)
5	FEC	I	1807[A]	1	40,56,56	1.22	4 (10%)	42,90,90	1.93	13 (30%)
3	SO4	G	1606	-	4,4,4	0.24	0	6,6,6	0.71	0
3	SO4	E	1304	1	4,4,4	1.92	1 (25%)	6,6,6	0.93	0
3	SO4	H	1701	-	4,4,4	1.84	1 (25%)	6,6,6	0.84	0
3	SO4	L	2103	1	4,4,4	1.94	1 (25%)	6,6,6	0.86	0
3	SO4	J	1906	-	4,4,4	0.16	0	6,6,6	0.95	0
5	FEC	B	1107[B]	1	40,56,56	1.21	3 (7%)	42,90,90	2.01	11 (26%)
3	SO4	E	1406	-	4,4,4	0.30	0	6,6,6	1.22	1 (16%)
3	SO4	M	2201	-	4,4,4	1.89	1 (25%)	6,6,6	0.93	0
3	SO4	I	1803	-	4,4,4	0.33	0	6,6,6	0.49	0
3	SO4	E	1401	-	4,4,4	1.92	1 (25%)	6,6,6	0.96	0
5	FEC	M	2207[A]	1	40,56,56	1.26	4 (10%)	42,90,90	1.74	10 (23%)
4	GOL	C	1210	-	5,5,5	4.37	5 (100%)	5,5,5	4.98	3 (60%)
3	SO4	C	1203	-	4,4,4	0.40	0	6,6,6	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	FEC	G	1608[A]	1	40,56,56	1.22	4 (10%)	42,90,90	1.83	14 (33%)
4	GOL	G	1610	-	5,5,5	4.53	5 (100%)	5,5,5	5.68	3 (60%)
3	SO4	A	1006	-	4,4,4	0.24	0	6,6,6	1.10	0
4	GOL	N	2310	-	5,5,5	4.51	5 (100%)	5,5,5	5.50	3 (60%)
3	SO4	J	1901	-	4,4,4	1.89	1 (25%)	6,6,6	0.84	0
4	GOL	B	1011	-	5,5,5	4.62	5 (100%)	5,5,5	4.00	3 (60%)
3	SO4	K	2006	-	4,4,4	0.17	0	6,6,6	0.67	0
3	SO4	N	2301	-	4,4,4	1.94	1 (25%)	6,6,6	0.81	0
3	SO4	I	1802	3	4,4,4	1.96	2 (50%)	6,6,6	0.79	0
4	GOL	O	2410	-	5,5,5	4.40	5 (100%)	5,5,5	4.82	3 (60%)
4	GOL	H	1814	-	5,5,5	4.64	5 (100%)	5,5,5	4.75	3 (60%)
5	FEC	P	2507[B]	1	40,56,56	1.19	4 (10%)	42,90,90	2.08	13 (30%)
3	SO4	K	2003	-	4,4,4	1.91	1 (25%)	6,6,6	0.92	0
5	FEC	B	1107[A]	1	40,56,56	1.21	3 (7%)	42,90,90	1.93	12 (28%)
3	SO4	G	1607	-	4,4,4	0.34	0	6,6,6	0.49	0
4	GOL	A	1010	-	5,5,5	4.64	5 (100%)	5,5,5	5.84	3 (60%)
5	FEC	D	1311[B]	1	40,56,56	1.23	4 (10%)	42,90,90	1.69	9 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	K	2011	-	-	2/4/4/4	-
5	FEC	G	1608[A]	1	-	10/20/120/120	-
4	GOL	D	1211	-	-	3/4/4/4	-
4	GOL	G	1611	-	-	2/4/4/4	-
4	GOL	G	1610	-	-	3/4/4/4	-
4	GOL	I	1713	-	-	3/4/4/4	-
4	GOL	I	1810	1	-	3/4/4/4	-
5	FEC	G	1608[B]	1	-	9/20/120/120	-
4	GOL	N	2310	-	-	4/4/4/4	-
4	GOL	F	1510	-	-	2/4/4/4	-
4	GOL	F	1512	-	-	2/4/4/4	-
4	GOL	E	1411	-	-	4/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	M	2210	1	-	2/4/4/4	-
4	GOL	H	1710	-	-	2/4/4/4	-
4	GOL	E	1410	-	-	2/4/4/4	-
4	GOL	B	1011	-	-	2/4/4/4	-
5	FEC	F	1507[A]	1	-	8/20/120/120	-
5	FEC	I	1807[A]	1	-	10/20/120/120	-
4	GOL	J	1910	-	-	2/4/4/4	-
5	FEC	I	1807[B]	1	-	13/20/120/120	-
5	FEC	L	2108[A]	1	-	9/20/120/120	-
4	GOL	O	2411	-	-	4/4/4/4	-
5	FEC	F	1507[B]	1	-	6/20/120/120	-
4	GOL	J	1811	-	-	3/4/4/4	-
5	FEC	L	2108[B]	1	-	9/20/120/120	-
5	FEC	P	2507[A]	1	-	8/20/120/120	-
4	GOL	O	2410	-	-	3/4/4/4	-
4	GOL	H	1814	-	-	3/4/4/4	-
5	FEC	P	2507[B]	1	-	10/20/120/120	-
5	FEC	B	1107[A]	1	-	9/20/120/120	-
4	GOL	B	1110	-	-	2/4/4/4	-
4	GOL	M	2211	-	-	2/4/4/4	-
4	GOL	P	2510	-	-	2/4/4/4	-
5	FEC	B	1107[B]	1	-	8/20/120/120	-
5	FEC	D	1311[A]	1	-	10/20/120/120	-
4	GOL	A	1010	-	-	2/4/4/4	-
6	3PY	D	1310	1	-	0/1/4/6	-
5	FEC	D	1311[B]	1	-	8/20/120/120	-
5	FEC	M	2207[A]	1	-	10/20/120/120	-
5	FEC	M	2207[B]	1	-	8/20/120/120	-
4	GOL	C	1210	-	-	2/4/4/4	-

All (213) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1310	3PY	C3-C2	-20.42	1.21	1.51
6	D	1310	3PY	O1-C1	17.86	1.63	1.22
4	A	1010	GOL	C3-C2	-7.61	1.20	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1710	GOL	C3-C2	-7.43	1.21	1.51
6	D	1310	3PY	O3-C2	7.39	1.35	1.23
4	J	1811	GOL	C3-C2	-7.38	1.21	1.51
4	G	1610	GOL	C3-C2	-7.35	1.21	1.51
4	N	2310	GOL	C3-C2	-7.31	1.21	1.51
4	D	1211	GOL	C3-C2	-7.28	1.21	1.51
4	I	1713	GOL	C3-C2	-7.26	1.21	1.51
4	K	2011	GOL	C3-C2	-7.25	1.21	1.51
4	E	1410	GOL	C3-C2	-7.22	1.22	1.51
4	C	1210	GOL	C3-C2	-7.22	1.22	1.51
4	H	1814	GOL	C3-C2	-7.22	1.22	1.51
4	B	1011	GOL	C3-C2	-7.21	1.22	1.51
4	J	1910	GOL	C3-C2	-7.20	1.22	1.51
4	M	2211	GOL	C3-C2	-7.20	1.22	1.51
4	P	2510	GOL	C3-C2	-7.18	1.22	1.51
4	M	2210	GOL	C3-C2	-7.17	1.22	1.51
4	O	2410	GOL	C3-C2	-7.17	1.22	1.51
4	B	1110	GOL	C3-C2	-7.15	1.22	1.51
4	G	1611	GOL	C3-C2	-7.08	1.22	1.51
4	F	1512	GOL	C3-C2	-7.08	1.22	1.51
4	F	1510	GOL	C3-C2	-7.02	1.22	1.51
4	E	1411	GOL	C3-C2	-7.01	1.22	1.51
4	O	2411	GOL	C3-C2	-6.88	1.23	1.51
4	I	1810	GOL	C3-C2	-6.86	1.23	1.51
6	D	1310	3PY	O4-C3	5.03	1.59	1.41
4	B	1011	GOL	O1-C1	4.89	1.63	1.42
4	F	1510	GOL	O1-C1	4.80	1.62	1.42
4	A	1010	GOL	O1-C1	4.77	1.62	1.42
4	N	2310	GOL	O1-C1	4.75	1.62	1.42
4	O	2411	GOL	O1-C1	4.74	1.62	1.42
4	H	1710	GOL	O1-C1	4.73	1.62	1.42
4	H	1814	GOL	O1-C1	4.71	1.62	1.42
4	M	2210	GOL	O1-C1	4.70	1.62	1.42
4	E	1411	GOL	O1-C1	4.69	1.62	1.42
4	D	1211	GOL	O1-C1	4.68	1.62	1.42
4	J	1811	GOL	O1-C1	4.63	1.62	1.42
4	M	2211	GOL	O1-C1	4.62	1.61	1.42
4	G	1611	GOL	O1-C1	4.58	1.61	1.42
4	F	1512	GOL	O1-C1	4.55	1.61	1.42
4	J	1910	GOL	O1-C1	4.54	1.61	1.42
4	I	1810	GOL	O1-C1	4.51	1.61	1.42
4	G	1610	GOL	O1-C1	4.50	1.61	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1410	GOL	O1-C1	4.50	1.61	1.42
4	B	1110	GOL	O1-C1	4.49	1.61	1.42
4	K	2011	GOL	O1-C1	4.46	1.61	1.42
4	P	2510	GOL	O1-C1	4.40	1.61	1.42
4	I	1713	GOL	O1-C1	4.40	1.61	1.42
4	O	2410	GOL	O1-C1	4.25	1.60	1.42
4	C	1210	GOL	O1-C1	4.25	1.60	1.42
4	E	1410	GOL	O3-C3	4.02	1.59	1.42
4	G	1611	GOL	O3-C3	3.99	1.59	1.42
4	J	1910	GOL	O3-C3	3.93	1.59	1.42
4	I	1810	GOL	O3-C3	3.86	1.58	1.42
4	F	1512	GOL	O3-C3	3.86	1.58	1.42
4	E	1411	GOL	O3-C3	3.86	1.58	1.42
4	M	2210	GOL	O3-C3	3.86	1.58	1.42
4	H	1814	GOL	O3-C3	3.83	1.58	1.42
4	B	1011	GOL	O3-C3	3.82	1.58	1.42
4	B	1110	GOL	O3-C3	3.82	1.58	1.42
4	O	2411	GOL	O3-C3	3.75	1.58	1.42
4	I	1713	GOL	O3-C3	3.75	1.58	1.42
4	M	2211	GOL	O3-C3	3.67	1.57	1.42
4	O	2410	GOL	O3-C3	3.66	1.57	1.42
4	P	2510	GOL	O3-C3	3.66	1.57	1.42
3	B	1104	SO4	O1-S	3.65	1.65	1.46
3	G	1603	SO4	O1-S	3.64	1.65	1.46
4	K	2011	GOL	O3-C3	3.60	1.57	1.42
4	A	1010	GOL	O3-C3	3.59	1.57	1.42
4	F	1510	GOL	O3-C3	3.57	1.57	1.42
3	F	1501	SO4	O1-S	3.56	1.65	1.46
4	C	1210	GOL	O3-C3	3.54	1.57	1.42
4	J	1811	GOL	O3-C3	3.53	1.57	1.42
3	D	1301	SO4	O1-S	3.52	1.65	1.46
4	D	1211	GOL	O3-C3	3.52	1.57	1.42
4	N	2310	GOL	O3-C3	3.49	1.57	1.42
3	L	2102	SO4	O1-S	3.48	1.64	1.46
3	L	2103	SO4	O1-S	3.48	1.64	1.46
3	K	1504	SO4	O1-S	3.47	1.64	1.46
4	H	1710	GOL	O3-C3	3.47	1.57	1.42
3	L	2107	SO4	O1-S	3.46	1.64	1.46
3	N	2301	SO4	O1-S	3.45	1.64	1.46
3	E	1401	SO4	O1-S	3.45	1.64	1.46
3	C	1201	SO4	O1-S	3.45	1.64	1.46
3	E	1304	SO4	O1-S	3.44	1.64	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1610	GOL	O3-C3	3.41	1.56	1.42
3	F	1502	SO4	O1-S	3.39	1.64	1.46
3	P	2501	SO4	O1-S	3.39	1.64	1.46
3	K	2003	SO4	O1-S	3.38	1.64	1.46
3	K	2001	SO4	O1-S	3.38	1.64	1.46
3	I	1801	SO4	O1-S	3.38	1.64	1.46
3	J	1904	SO4	O1-S	3.37	1.64	1.46
3	J	1901	SO4	O1-S	3.36	1.64	1.46
3	L	2101	SO4	O1-S	3.36	1.64	1.46
3	B	1101	SO4	O1-S	3.35	1.64	1.46
3	A	1004	SO4	O1-S	3.34	1.64	1.46
3	M	2201	SO4	O1-S	3.30	1.63	1.46
3	I	1802	SO4	O1-S	3.30	1.63	1.46
3	H	1701	SO4	O1-S	3.21	1.63	1.46
4	H	1814	GOL	O2-C2	-3.16	1.34	1.43
4	B	1011	GOL	C1-C2	-3.08	1.39	1.51
4	F	1512	GOL	C1-C2	-3.08	1.39	1.51
3	A	1001	SO4	O1-S	3.07	1.62	1.46
4	G	1610	GOL	C1-C2	-2.96	1.39	1.51
4	H	1814	GOL	C1-C2	-2.96	1.39	1.51
4	J	1910	GOL	C1-C2	-2.95	1.39	1.51
4	E	1410	GOL	C1-C2	-2.93	1.39	1.51
4	C	1210	GOL	C1-C2	-2.90	1.39	1.51
4	A	1010	GOL	C1-C2	-2.88	1.39	1.51
4	I	1810	GOL	C1-C2	-2.88	1.39	1.51
5	L	2108[B]	FEC	CMB-C2B	2.86	1.55	1.50
4	O	2411	GOL	C1-C2	-2.86	1.40	1.51
5	M	2207[B]	FEC	CMD-C2D	2.86	1.55	1.50
4	M	2211	GOL	C1-C2	-2.85	1.40	1.51
4	B	1110	GOL	O2-C2	-2.83	1.34	1.43
4	I	1713	GOL	C1-C2	-2.82	1.40	1.51
5	B	1107[B]	FEC	CMD-C2D	2.81	1.55	1.50
4	G	1610	GOL	O2-C2	-2.81	1.35	1.43
5	M	2207[A]	FEC	CMB-C2B	2.80	1.55	1.50
4	B	1110	GOL	C1-C2	-2.78	1.40	1.51
4	F	1512	GOL	O2-C2	-2.78	1.35	1.43
4	D	1211	GOL	C1-C2	-2.77	1.40	1.51
4	P	2510	GOL	O2-C2	-2.76	1.35	1.43
4	N	2310	GOL	C1-C2	-2.76	1.40	1.51
4	H	1710	GOL	O2-C2	-2.76	1.35	1.43
4	P	2510	GOL	C1-C2	-2.75	1.40	1.51
4	O	2410	GOL	C1-C2	-2.73	1.40	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	2108[A]	FEC	CMB-C2B	2.72	1.55	1.50
5	B	1107[A]	FEC	CMD-C2D	2.72	1.55	1.50
4	J	1910	GOL	O2-C2	-2.72	1.35	1.43
5	G	1608[B]	FEC	CMB-C2B	2.72	1.55	1.50
5	L	2108[A]	FEC	CMD-C2D	2.71	1.55	1.50
5	P	2507[A]	FEC	CMD-C2D	2.71	1.55	1.50
4	M	2211	GOL	O2-C2	-2.70	1.35	1.43
4	E	1411	GOL	O2-C2	-2.70	1.35	1.43
4	M	2210	GOL	C1-C2	-2.68	1.40	1.51
4	F	1510	GOL	C1-C2	-2.68	1.40	1.51
5	D	1311[A]	FEC	CMD-C2D	2.67	1.54	1.50
5	D	1311[B]	FEC	CMB-C2B	2.66	1.54	1.50
5	D	1311[A]	FEC	CMB-C2B	2.64	1.54	1.50
5	F	1507[A]	FEC	CMD-C2D	2.63	1.54	1.50
5	I	1807[B]	FEC	CMB-C2B	2.63	1.54	1.50
4	J	1811	GOL	O2-C2	-2.63	1.35	1.43
5	G	1608[A]	FEC	CMD-C2D	2.63	1.54	1.50
4	J	1811	GOL	C1-C2	-2.61	1.41	1.51
5	P	2507[A]	FEC	CMB-C2B	2.61	1.54	1.50
5	L	2108[B]	FEC	CMD-C2D	2.59	1.54	1.50
6	D	1310	3PY	C1-C2	-2.59	1.39	1.46
4	F	1510	GOL	O2-C2	-2.59	1.35	1.43
5	I	1807[A]	FEC	CMD-C2D	2.59	1.54	1.50
4	K	2011	GOL	O2-C2	-2.57	1.35	1.43
5	F	1507[B]	FEC	CMD-C2D	2.56	1.54	1.50
5	I	1807[B]	FEC	CMD-C2D	2.55	1.54	1.50
4	B	1011	GOL	O2-C2	-2.55	1.35	1.43
5	G	1608[A]	FEC	CMB-C2B	2.54	1.54	1.50
5	D	1311[B]	FEC	CMD-C2D	2.54	1.54	1.50
5	I	1807[A]	FEC	CMB-C2B	2.54	1.54	1.50
4	I	1713	GOL	O2-C2	-2.53	1.35	1.43
4	K	2011	GOL	C1-C2	-2.52	1.41	1.51
4	D	1211	GOL	O2-C2	-2.52	1.35	1.43
5	B	1107[A]	FEC	CMB-C2B	2.50	1.54	1.50
4	O	2410	GOL	O2-C2	-2.49	1.35	1.43
4	M	2210	GOL	O2-C2	-2.47	1.36	1.43
5	M	2207[A]	FEC	CMD-C2D	2.47	1.54	1.50
5	G	1608[B]	FEC	CMD-C2D	2.46	1.54	1.50
5	F	1507[A]	FEC	CAD-C3D	2.46	1.55	1.51
4	N	2310	GOL	O2-C2	-2.46	1.36	1.43
5	F	1507[A]	FEC	CMB-C2B	2.43	1.54	1.50
5	M	2207[B]	FEC	CMB-C2B	2.43	1.54	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1411	GOL	C1-C2	-2.43	1.41	1.51
5	B	1107[B]	FEC	CMB-C2B	2.43	1.54	1.50
5	B	1107[B]	FEC	CAB-C3B	2.40	1.55	1.51
5	D	1311[A]	FEC	CAB-C3B	2.39	1.55	1.51
4	A	1010	GOL	O2-C2	-2.39	1.36	1.43
5	F	1507[B]	FEC	CMB-C2B	2.39	1.54	1.50
5	F	1507[A]	FEC	CAB-C3B	2.38	1.55	1.51
5	P	2507[B]	FEC	CMD-C2D	2.38	1.54	1.50
5	M	2207[B]	FEC	CAB-C3B	2.36	1.55	1.51
5	P	2507[B]	FEC	CMB-C2B	2.36	1.54	1.50
4	H	1710	GOL	C1-C2	-2.35	1.42	1.51
4	E	1410	GOL	O2-C2	-2.35	1.36	1.43
5	L	2108[B]	FEC	CAD-C3D	2.34	1.55	1.51
5	F	1507[B]	FEC	CAD-C3D	2.34	1.55	1.51
4	O	2411	GOL	O2-C2	-2.32	1.36	1.43
5	M	2207[A]	FEC	CAB-C3B	2.29	1.55	1.51
5	M	2207[B]	FEC	CAD-C3D	2.29	1.55	1.51
4	I	1810	GOL	O2-C2	-2.27	1.36	1.43
4	G	1611	GOL	C1-C2	-2.27	1.42	1.51
5	L	2108[B]	FEC	CAB-C3B	2.27	1.55	1.51
5	D	1311[B]	FEC	CAB-C3B	2.26	1.55	1.51
5	G	1608[B]	FEC	CAB-C3B	2.25	1.55	1.51
5	I	1807[A]	FEC	CAB-C3B	2.24	1.55	1.51
5	D	1311[A]	FEC	CAD-C3D	2.23	1.55	1.51
5	G	1608[A]	FEC	CAB-C3B	2.21	1.54	1.51
5	I	1807[A]	FEC	CAD-C3D	2.21	1.54	1.51
5	D	1311[B]	FEC	CAD-C3D	2.19	1.54	1.51
5	P	2507[A]	FEC	CAD-C3D	2.18	1.54	1.51
5	B	1107[A]	FEC	CAD-C3D	2.17	1.54	1.51
5	L	2108[A]	FEC	CAB-C3B	2.17	1.54	1.51
5	F	1507[B]	FEC	CAB-C3B	2.17	1.54	1.51
5	P	2507[B]	FEC	CAD-C3D	2.15	1.54	1.51
5	G	1608[A]	FEC	CAD-C3D	2.13	1.54	1.51
5	I	1807[B]	FEC	CAD-C3D	2.09	1.54	1.51
5	G	1608[B]	FEC	CAD-C3D	2.09	1.54	1.51
4	C	1210	GOL	O2-C2	-2.08	1.37	1.43
5	P	2507[B]	FEC	CAB-C3B	2.07	1.54	1.51
5	M	2207[A]	FEC	CAD-C3D	2.06	1.54	1.51
5	P	2507[A]	FEC	CAB-C3B	2.05	1.54	1.51
4	G	1611	GOL	O2-C2	-2.04	1.37	1.43
5	I	1807[B]	FEC	CAB-C3B	2.03	1.54	1.51
3	I	1802	SO4	O3-S	-2.03	1.31	1.47

All (274) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	1310	3PY	O4-C3-C2	12.04	145.08	112.66
4	A	1010	GOL	O3-C3-C2	11.00	162.95	110.20
4	I	1713	GOL	O3-C3-C2	10.39	160.02	110.20
4	N	2310	GOL	O3-C3-C2	10.15	158.86	110.20
4	J	1811	GOL	O3-C3-C2	10.09	158.60	110.20
4	G	1610	GOL	O3-C3-C2	9.99	158.10	110.20
4	H	1710	GOL	O3-C3-C2	9.89	157.64	110.20
6	D	1310	3PY	O3-C2-C3	8.84	140.63	116.92
4	C	1210	GOL	O3-C3-C2	8.65	151.66	110.20
4	J	1910	GOL	O3-C3-C2	8.56	151.24	110.20
4	O	2410	GOL	O3-C3-C2	8.54	151.14	110.20
4	K	2011	GOL	O3-C3-C2	8.43	150.63	110.20
4	D	1211	GOL	O3-C3-C2	8.31	150.06	110.20
4	F	1510	GOL	O3-C3-C2	8.12	149.16	110.20
6	D	1310	3PY	O3-C2-C1	-8.09	108.23	123.20
4	G	1611	GOL	O3-C3-C2	7.87	147.96	110.20
4	M	2211	GOL	O3-C3-C2	7.85	147.84	110.20
5	P	2507[B]	FEC	CBC-CAC-C2C	7.77	125.70	112.60
4	H	1814	GOL	O3-C3-C2	7.72	147.22	110.20
4	P	2510	GOL	O3-C3-C2	7.71	147.15	110.20
5	P	2507[A]	FEC	CBC-CAC-C2C	7.70	125.58	112.60
4	M	2210	GOL	O3-C3-C2	7.68	147.05	110.20
4	E	1410	GOL	O3-C3-C2	7.56	146.43	110.20
5	B	1107[B]	FEC	CBC-CAC-C2C	7.48	125.21	112.60
4	B	1110	GOL	O3-C3-C2	7.45	145.90	110.20
5	I	1807[B]	FEC	CBC-CAC-C2C	7.37	125.02	112.60
5	D	1311[A]	FEC	CBC-CAC-C2C	7.30	124.91	112.60
4	H	1710	GOL	O2-C2-C3	7.13	140.53	109.12
4	G	1610	GOL	O2-C2-C3	7.08	140.32	109.12
4	O	2411	GOL	O3-C3-C2	6.90	143.29	110.20
4	E	1411	GOL	O3-C3-C2	6.86	143.11	110.20
4	P	2510	GOL	O2-C2-C3	6.58	138.08	109.12
5	I	1807[A]	FEC	CBC-CAC-C2C	6.55	123.65	112.60
4	I	1810	GOL	O3-C3-C2	6.49	141.33	110.20
4	F	1510	GOL	O2-C2-C3	6.44	137.49	109.12
5	F	1507[B]	FEC	CBC-CAC-C2C	6.41	123.41	112.60
4	H	1814	GOL	O2-C2-C3	6.40	137.33	109.12
5	B	1107[A]	FEC	CBC-CAC-C2C	6.38	123.36	112.60
4	B	1011	GOL	O3-C3-C2	6.35	140.64	110.20
5	L	2108[B]	FEC	CBC-CAC-C2C	6.33	123.28	112.60
4	B	1110	GOL	O2-C2-C3	6.18	136.36	109.12
4	K	2011	GOL	O2-C2-C3	6.08	135.90	109.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	N	2310	GOL	O2-C2-C3	6.05	135.78	109.12
4	I	1713	GOL	O2-C2-C3	6.03	135.68	109.12
4	J	1811	GOL	O2-C2-C3	6.00	135.55	109.12
4	A	1010	GOL	O2-C2-C3	5.99	135.51	109.12
4	C	1210	GOL	O2-C2-C3	5.97	135.44	109.12
4	M	2211	GOL	O2-C2-C3	5.95	135.34	109.12
5	L	2108[A]	FEC	CBC-CAC-C2C	5.90	122.55	112.60
4	E	1411	GOL	O2-C2-C3	5.88	135.01	109.12
4	J	1910	GOL	O2-C2-C3	5.78	134.56	109.12
4	B	1011	GOL	O2-C2-C3	5.74	134.38	109.12
4	M	2210	GOL	O2-C2-C3	5.73	134.38	109.12
5	G	1608[B]	FEC	CBC-CAC-C2C	5.73	122.26	112.60
4	D	1211	GOL	O2-C2-C3	5.66	134.07	109.12
4	F	1512	GOL	O3-C3-C2	5.66	137.32	110.20
4	F	1512	GOL	O2-C2-C3	5.42	133.00	109.12
4	O	2410	GOL	O2-C2-C3	5.35	132.70	109.12
4	G	1611	GOL	O2-C2-C3	5.35	132.69	109.12
5	G	1608[A]	FEC	CBC-CAC-C2C	5.21	121.38	112.60
4	E	1410	GOL	O2-C2-C3	4.88	130.63	109.12
5	F	1507[A]	FEC	CBC-CAC-C2C	4.68	120.50	112.60
4	I	1810	GOL	O2-C2-C3	4.66	129.67	109.12
4	O	2411	GOL	O2-C2-C3	4.65	129.60	109.12
5	M	2207[A]	FEC	CBC-CAC-C2C	4.60	120.36	112.60
5	M	2207[B]	FEC	CBC-CAC-C2C	4.58	120.32	112.60
3	A	1105	SO4	O4-S-O1	4.25	131.51	109.31
3	A	1008	SO4	O4-S-O1	4.25	131.48	109.31
3	B	1005	SO4	O4-S-O1	4.25	131.47	109.31
5	D	1311[B]	FEC	CBA-CAA-C3A	4.13	119.56	112.60
5	F	1507[B]	FEC	C4B-CHC-C1C	4.00	129.48	118.67
5	D	1311[B]	FEC	CBC-CAC-C2C	3.96	119.28	112.60
5	G	1608[B]	FEC	C4B-CHC-C1C	3.82	128.99	118.67
4	A	1010	GOL	O1-C1-C2	3.59	127.40	110.20
4	C	1210	GOL	O1-C1-C2	3.57	127.30	110.20
4	E	1410	GOL	O1-C1-C2	3.53	127.14	110.20
5	D	1311[A]	FEC	C4B-CHC-C1C	3.53	128.21	118.67
5	B	1107[B]	FEC	CAB-CBB-CGB	3.51	121.16	113.60
6	D	1310	3PY	O1-C1-C2	-3.44	116.42	124.09
4	O	2410	GOL	O1-C1-C2	3.40	126.52	110.20
4	I	1713	GOL	O1-C1-C2	3.38	126.41	110.20
4	H	1814	GOL	O1-C1-C2	3.37	126.35	110.20
5	P	2507[B]	FEC	C4B-CHC-C1C	3.37	127.78	118.67
3	A	1105	SO4	O4-S-O3	-3.37	94.70	109.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	1910	GOL	O1-C1-C2	3.36	126.31	110.20
3	B	1005	SO4	O4-S-O3	-3.36	94.73	109.06
3	A	1008	SO4	O4-S-O3	-3.35	94.77	109.06
5	I	1807[A]	FEC	CBA-CAA-C3A	3.30	118.17	112.60
4	N	2310	GOL	O1-C1-C2	3.29	125.99	110.20
5	I	1807[B]	FEC	CBB-CAB-C3B	3.27	121.63	112.62
5	B	1107[A]	FEC	CBA-CAA-C3A	3.26	118.10	112.60
4	I	1810	GOL	O1-C1-C2	3.24	125.73	110.20
4	H	1710	GOL	O1-C1-C2	3.21	125.61	110.20
5	L	2108[A]	FEC	C4B-CHC-C1C	3.21	127.36	118.67
5	B	1107[B]	FEC	C4B-CHC-C1C	3.20	127.33	118.67
5	B	1107[A]	FEC	C4B-CHC-C1C	3.17	127.24	118.67
5	I	1807[B]	FEC	C4B-CHC-C1C	3.17	127.23	118.67
5	P	2507[B]	FEC	CBA-CAA-C3A	3.15	117.91	112.60
4	G	1610	GOL	O1-C1-C2	3.13	125.20	110.20
5	G	1608[A]	FEC	C4B-CHC-C1C	3.12	127.11	118.67
5	D	1311[A]	FEC	CBB-CAB-C3B	3.08	121.11	112.62
5	M	2207[A]	FEC	C4B-CHC-C1C	3.02	126.83	118.67
5	I	1807[A]	FEC	C4B-CHC-C1C	3.01	126.80	118.67
5	I	1807[B]	FEC	CBA-CAA-C3A	2.92	117.52	112.60
5	G	1608[B]	FEC	CBB-CAB-C3B	2.88	120.55	112.62
5	B	1107[A]	FEC	CBB-CAB-C3B	2.87	120.53	112.62
5	P	2507[A]	FEC	C4B-CHC-C1C	2.86	126.41	118.67
5	P	2507[A]	FEC	CBA-CAA-C3A	2.86	117.42	112.60
5	I	1807[A]	FEC	CBB-CAB-C3B	2.84	120.45	112.62
5	P	2507[B]	FEC	C3D-C4D-ND	-2.81	108.92	114.98
5	P	2507[A]	FEC	CBB-CAB-C3B	2.81	120.36	112.62
5	G	1608[B]	FEC	CAB-CBB-CGB	2.80	119.63	113.60
5	L	2108[B]	FEC	C4B-CHC-C1C	2.76	126.12	118.67
5	F	1507[A]	FEC	C4B-CHC-C1C	2.74	126.09	118.67
4	F	1512	GOL	O1-C1-C2	2.72	123.22	110.20
5	P	2507[B]	FEC	CBB-CAB-C3B	2.71	120.08	112.62
5	I	1807[B]	FEC	CAB-C3B-C2B	2.71	132.92	127.88
5	D	1311[B]	FEC	C3D-C4D-ND	-2.70	109.15	114.98
5	B	1107[A]	FEC	CMC-C3C-C2C	2.69	130.02	124.94
5	B	1107[B]	FEC	CBA-CAA-C3A	2.68	117.13	112.60
4	D	1211	GOL	O1-C1-C2	2.68	123.04	110.20
5	M	2207[A]	FEC	CBA-CAA-C3A	2.68	117.12	112.60
5	F	1507[B]	FEC	CMA-C2A-C3A	2.67	129.98	124.94
5	D	1311[A]	FEC	CMA-C2A-C3A	2.67	129.97	124.94
4	K	2011	GOL	O1-C1-C2	2.66	122.98	110.20
5	L	2108[A]	FEC	CBB-CAB-C3B	2.66	119.96	112.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	1506	SO4	O4-S-O1	2.66	123.20	109.31
5	B	1107[B]	FEC	C1D-CHD-C4C	2.66	125.86	118.67
5	G	1608[B]	FEC	CMC-C3C-C2C	2.65	129.94	124.94
4	M	2211	GOL	O1-C1-C2	2.65	122.89	110.20
5	L	2108[A]	FEC	CMA-C2A-C3A	2.64	129.93	124.94
4	P	2510	GOL	O1-C1-C2	2.63	122.81	110.20
5	M	2207[B]	FEC	C4B-CHC-C1C	2.62	125.76	118.67
5	G	1608[B]	FEC	CBA-CAA-C3A	2.62	117.02	112.60
4	J	1811	GOL	O1-C1-C2	2.62	122.75	110.20
5	M	2207[B]	FEC	C1D-CHD-C4C	2.61	125.74	118.67
4	O	2411	GOL	O1-C1-C2	2.60	122.66	110.20
5	P	2507[A]	FEC	C4D-CHA-C1A	2.60	125.69	118.67
5	P	2507[A]	FEC	C1B-CHB-C4A	2.59	125.66	118.67
5	B	1107[B]	FEC	C3D-C4D-ND	-2.58	109.42	114.98
5	M	2207[B]	FEC	C3B-C4B-NB	-2.57	109.44	114.98
5	B	1107[A]	FEC	C4D-CHA-C1A	2.57	125.62	118.67
5	P	2507[B]	FEC	C4D-CHA-C1A	2.57	125.61	118.67
5	P	2507[B]	FEC	CMA-C2A-C3A	2.56	129.78	124.94
5	B	1107[B]	FEC	C1B-CHB-C4A	2.56	125.60	118.67
5	I	1807[A]	FEC	C4D-CHA-C1A	2.55	125.57	118.67
5	D	1311[B]	FEC	C4B-CHC-C1C	2.54	125.55	118.67
5	I	1807[B]	FEC	C3D-C4D-ND	-2.54	109.50	114.98
5	D	1311[B]	FEC	C4D-CHA-C1A	2.54	125.54	118.67
5	L	2108[A]	FEC	C3D-C4D-ND	-2.53	109.51	114.98
5	L	2108[B]	FEC	C3D-C4D-ND	-2.53	109.52	114.98
5	F	1507[A]	FEC	O1C-CGC-CBC	-2.52	114.98	123.08
5	G	1608[A]	FEC	CBA-CAA-C3A	2.52	116.85	112.60
5	F	1507[B]	FEC	C4D-CHA-C1A	2.52	125.47	118.67
4	B	1011	GOL	O1-C1-C2	2.51	122.26	110.20
5	I	1807[B]	FEC	C4D-CHA-C1A	2.51	125.47	118.67
5	G	1608[B]	FEC	CMA-C2A-C3A	2.51	129.67	124.94
5	I	1807[A]	FEC	C3D-C4D-ND	-2.50	109.59	114.98
5	L	2108[B]	FEC	C1B-CHB-C4A	2.49	125.41	118.67
5	G	1608[A]	FEC	C3D-C4D-ND	-2.49	109.61	114.98
5	F	1507[A]	FEC	C4D-CHA-C1A	2.49	125.41	118.67
5	M	2207[A]	FEC	C3D-C4D-ND	-2.49	109.62	114.98
5	I	1807[A]	FEC	CAB-CBB-CGB	2.48	118.94	113.60
5	M	2207[A]	FEC	CMA-C2A-C3A	2.48	129.62	124.94
5	F	1507[B]	FEC	C3D-C4D-ND	-2.47	109.66	114.98
5	M	2207[A]	FEC	O1C-CGC-CBC	-2.46	115.17	123.08
5	F	1507[B]	FEC	CBB-CAB-C3B	2.46	119.38	112.62
5	F	1507[A]	FEC	CMC-C3C-C2C	2.45	129.56	124.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	2207[B]	FEC	CMA-C2A-C3A	2.44	129.53	124.94
4	F	1510	GOL	O1-C1-C2	2.43	121.85	110.20
5	D	1311[B]	FEC	C1D-CHD-C4C	2.43	125.23	118.67
5	M	2207[A]	FEC	C1D-CHD-C4C	2.43	125.23	118.67
5	P	2507[B]	FEC	C1D-CHD-C4C	2.42	125.22	118.67
4	B	1110	GOL	O1-C1-C2	2.41	121.76	110.20
5	D	1311[A]	FEC	C4D-CHA-C1A	2.41	125.19	118.67
3	E	1406	SO4	O3-S-O1	-2.41	96.73	109.31
5	G	1608[B]	FEC	C3D-C4D-ND	-2.41	109.78	114.98
5	P	2507[B]	FEC	O1D-CGD-CBD	-2.40	115.37	123.08
5	L	2108[B]	FEC	C3B-C4B-NB	-2.40	109.81	114.98
5	B	1107[A]	FEC	CMA-C2A-C3A	2.39	129.45	124.94
5	M	2207[A]	FEC	C1B-CHB-C4A	2.39	125.13	118.67
5	L	2108[A]	FEC	CMC-C3C-C2C	2.39	129.45	124.94
5	B	1107[A]	FEC	C3D-C4D-ND	-2.39	109.83	114.98
5	M	2207[B]	FEC	O1C-CGC-CBC	-2.39	115.41	123.08
5	F	1507[A]	FEC	C3D-C4D-ND	-2.37	109.86	114.98
5	G	1608[A]	FEC	CMC-C3C-C2C	2.37	129.42	124.94
5	I	1807[B]	FEC	CMA-C2A-C3A	2.37	129.42	124.94
5	D	1311[B]	FEC	O1C-CGC-CBC	-2.37	115.45	123.08
5	P	2507[A]	FEC	CMA-C2A-C3A	2.37	129.41	124.94
5	P	2507[A]	FEC	C3D-C4D-ND	-2.37	109.87	114.98
5	G	1608[A]	FEC	O1D-CGD-CBD	-2.37	115.48	123.08
5	L	2108[A]	FEC	C4D-CHA-C1A	2.36	125.05	118.67
5	G	1608[B]	FEC	C1B-CHB-C4A	2.35	125.03	118.67
5	P	2507[B]	FEC	CAB-C3B-C2B	2.35	132.25	127.88
5	G	1608[B]	FEC	O1C-CGC-CBC	-2.33	115.60	123.08
5	L	2108[A]	FEC	C1B-CHB-C4A	2.33	124.97	118.67
5	G	1608[A]	FEC	O1C-CGC-CBC	-2.32	115.62	123.08
5	L	2108[B]	FEC	CMA-C2A-C3A	2.30	129.28	124.94
4	E	1411	GOL	O1-C1-C2	2.30	121.23	110.20
5	D	1311[B]	FEC	C3B-C4B-NB	-2.29	110.03	114.98
5	M	2207[A]	FEC	C4D-CHA-C1A	2.29	124.86	118.67
5	D	1311[A]	FEC	C3D-C4D-ND	-2.29	110.05	114.98
5	F	1507[A]	FEC	CBA-CAA-C3A	2.29	116.46	112.60
5	I	1807[A]	FEC	O1C-CGC-CBC	-2.28	115.75	123.08
5	L	2108[A]	FEC	O1C-CGC-CBC	-2.28	115.75	123.08
5	D	1311[A]	FEC	C1D-CHD-C4C	2.28	124.83	118.67
5	I	1807[A]	FEC	CMA-C2A-C3A	2.27	129.22	124.94
5	F	1507[B]	FEC	O1D-CGD-CBD	-2.27	115.79	123.08
5	M	2207[B]	FEC	O2A-CGA-CBA	-2.26	115.82	123.08
5	B	1107[A]	FEC	C1B-CHB-C4A	2.26	124.78	118.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1107[B]	FEC	C4D-CHA-C1A	2.25	124.77	118.67
5	M	2207[A]	FEC	CBB-CAB-C3B	2.25	118.83	112.62
5	B	1107[B]	FEC	CMA-C2A-C3A	2.25	129.18	124.94
5	F	1507[B]	FEC	C1D-CHD-C4C	2.25	124.75	118.67
5	G	1608[B]	FEC	C3B-C4B-NB	-2.24	110.14	114.98
5	I	1807[B]	FEC	C1B-CHB-C4A	2.24	124.73	118.67
5	P	2507[B]	FEC	CAB-CBB-CGB	2.24	118.42	113.60
5	I	1807[B]	FEC	C1D-CHD-C4C	2.24	124.72	118.67
5	G	1608[A]	FEC	C4D-CHA-C1A	2.24	124.72	118.67
5	M	2207[B]	FEC	C4D-CHA-C1A	2.23	124.71	118.67
5	L	2108[B]	FEC	CBA-CAA-C3A	2.23	116.37	112.60
5	I	1807[B]	FEC	O2A-CGA-CBA	-2.23	115.92	123.08
5	F	1507[A]	FEC	CMA-C2A-C3A	2.23	129.14	124.94
5	F	1507[A]	FEC	C1B-CHB-C4A	2.22	124.68	118.67
6	D	1310	3PY	C3-C2-C1	-2.22	110.48	118.03
5	L	2108[A]	FEC	C3B-C4B-NB	-2.21	110.21	114.98
5	F	1507[A]	FEC	O2A-CGA-CBA	-2.21	115.97	123.08
5	L	2108[B]	FEC	C4D-CHA-C1A	2.21	124.64	118.67
5	P	2507[B]	FEC	O2A-CGA-CBA	-2.21	116.00	123.08
5	P	2507[A]	FEC	CMC-C3C-C2C	2.20	129.10	124.94
5	G	1608[B]	FEC	C4D-CHA-C1A	2.20	124.63	118.67
5	I	1807[A]	FEC	C1B-CHB-C4A	2.20	124.61	118.67
5	D	1311[B]	FEC	C1B-CHB-C4A	2.19	124.60	118.67
5	D	1311[A]	FEC	O2A-CGA-CBA	-2.19	116.04	123.08
5	G	1608[B]	FEC	C1D-CHD-C4C	2.19	124.59	118.67
5	M	2207[B]	FEC	CBD-CAD-C3D	2.19	118.65	112.62
5	D	1311[A]	FEC	C3B-C4B-NB	-2.18	110.27	114.98
5	F	1507[B]	FEC	C1B-CHB-C4A	2.18	124.57	118.67
5	P	2507[A]	FEC	C3B-C4B-NB	-2.18	110.28	114.98
5	G	1608[A]	FEC	O2C-CGC-O1C	2.18	128.73	123.30
5	B	1107[B]	FEC	CBD-CAD-C3D	2.18	118.61	112.62
5	D	1311[A]	FEC	O1C-CGC-CBC	-2.17	116.12	123.08
5	I	1807[A]	FEC	C1D-CHD-C4C	2.15	124.50	118.67
5	I	1807[A]	FEC	CMC-C3C-C2C	2.15	129.00	124.94
5	D	1311[A]	FEC	C1B-CHB-C4A	2.15	124.49	118.67
5	G	1608[A]	FEC	CMA-C2A-C3A	2.15	128.99	124.94
5	M	2207[B]	FEC	CAD-CBD-CGD	2.14	118.21	113.60
5	M	2207[B]	FEC	CBB-CAB-C3B	2.13	118.49	112.62
5	M	2207[B]	FEC	C3D-C4D-ND	-2.11	110.42	114.98
5	G	1608[A]	FEC	C1D-CHD-C4C	2.11	124.38	118.67
5	M	2207[B]	FEC	C1B-CHB-C4A	2.11	124.38	118.67
5	L	2108[B]	FEC	C1D-CHD-C4C	2.11	124.36	118.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1107[B]	FEC	O2A-CGA-CBA	-2.10	116.33	123.08
5	L	2108[A]	FEC	C1D-CHD-C4C	2.10	124.35	118.67
5	F	1507[A]	FEC	C3B-C4B-NB	-2.10	110.45	114.98
5	G	1608[A]	FEC	O2A-CGA-CBA	-2.09	116.36	123.08
5	F	1507[B]	FEC	O1C-CGC-CBC	-2.09	116.37	123.08
5	G	1608[A]	FEC	C3B-C4B-NB	-2.07	110.51	114.98
5	D	1311[A]	FEC	O2C-CGC-O1C	2.07	128.46	123.30
5	F	1507[A]	FEC	C1D-CHD-C4C	2.06	124.25	118.67
5	G	1608[A]	FEC	CBB-CAB-C3B	2.06	118.28	112.62
5	B	1107[A]	FEC	O1C-CGC-CBC	-2.04	116.53	123.08
5	I	1807[A]	FEC	C3B-C4B-NB	-2.04	110.59	114.98
5	B	1107[A]	FEC	O2A-CGA-CBA	-2.04	116.54	123.08
5	D	1311[A]	FEC	CMC-C3C-C2C	2.03	128.78	124.94
5	M	2207[B]	FEC	O2C-CGC-O1C	2.03	128.37	123.30
5	P	2507[B]	FEC	C1D-C2D-C3D	-2.03	106.92	108.61
5	P	2507[A]	FEC	CAB-C3B-C2B	2.03	131.65	127.88
4	G	1611	GOL	O1-C1-C2	2.02	119.87	110.20
5	F	1507[A]	FEC	CBB-CAB-C3B	2.01	118.17	112.62
5	G	1608[B]	FEC	O1D-CGD-CBD	-2.01	116.61	123.08
5	P	2507[A]	FEC	O2A-CGA-CBA	-2.01	116.62	123.08
5	I	1807[B]	FEC	C3B-C4B-NB	-2.01	110.65	114.98
5	B	1107[A]	FEC	C1D-CHD-C4C	2.00	124.08	118.67

There are no chirality outliers.

All (206) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1010	GOL	O1-C1-C2-C3
4	C	1210	GOL	O1-C1-C2-C3
4	E	1410	GOL	O1-C1-C2-C3
4	E	1411	GOL	O1-C1-C2-C3
4	G	1611	GOL	O1-C1-C2-C3
4	H	1814	GOL	O1-C1-C2-C3
4	I	1810	GOL	O1-C1-C2-C3
4	J	1811	GOL	C1-C2-C3-O3
4	J	1910	GOL	O1-C1-C2-C3
4	N	2310	GOL	O1-C1-C2-C3
4	N	2310	GOL	C1-C2-C3-O3
4	O	2410	GOL	O1-C1-C2-C3
4	O	2410	GOL	C1-C2-C3-O3
4	O	2411	GOL	C1-C2-C3-O3
5	B	1107[A]	FEC	C3C-C2C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	1107[A]	FEC	C1C-C2C-CAC-CBC
5	B	1107[B]	FEC	C3C-C2C-CAC-CBC
5	B	1107[B]	FEC	C1C-C2C-CAC-CBC
5	D	1311[A]	FEC	C3C-C2C-CAC-CBC
5	D	1311[A]	FEC	C1C-C2C-CAC-CBC
5	D	1311[B]	FEC	C3C-C2C-CAC-CBC
5	D	1311[B]	FEC	C1C-C2C-CAC-CBC
5	F	1507[A]	FEC	C3C-C2C-CAC-CBC
5	F	1507[A]	FEC	C1C-C2C-CAC-CBC
5	F	1507[B]	FEC	C3C-C2C-CAC-CBC
5	F	1507[B]	FEC	C1C-C2C-CAC-CBC
5	G	1608[A]	FEC	C3C-C2C-CAC-CBC
5	G	1608[A]	FEC	C1C-C2C-CAC-CBC
5	G	1608[B]	FEC	C3C-C2C-CAC-CBC
5	G	1608[B]	FEC	C1C-C2C-CAC-CBC
5	I	1807[A]	FEC	C3C-C2C-CAC-CBC
5	I	1807[A]	FEC	C1C-C2C-CAC-CBC
5	I	1807[B]	FEC	C3C-C2C-CAC-CBC
5	I	1807[B]	FEC	C1C-C2C-CAC-CBC
5	I	1807[B]	FEC	C4B-C3B-CAB-CBB
5	I	1807[B]	FEC	C2B-C3B-CAB-CBB
5	L	2108[A]	FEC	C3C-C2C-CAC-CBC
5	L	2108[A]	FEC	C1C-C2C-CAC-CBC
5	L	2108[B]	FEC	C3C-C2C-CAC-CBC
5	L	2108[B]	FEC	C1C-C2C-CAC-CBC
5	M	2207[A]	FEC	C3C-C2C-CAC-CBC
5	M	2207[A]	FEC	C1C-C2C-CAC-CBC
5	M	2207[B]	FEC	C3C-C2C-CAC-CBC
5	M	2207[B]	FEC	C1C-C2C-CAC-CBC
5	P	2507[A]	FEC	C3C-C2C-CAC-CBC
5	P	2507[A]	FEC	C1C-C2C-CAC-CBC
5	P	2507[B]	FEC	C3C-C2C-CAC-CBC
5	P	2507[B]	FEC	C1C-C2C-CAC-CBC
5	P	2507[B]	FEC	C4B-C3B-CAB-CBB
5	P	2507[B]	FEC	C2B-C3B-CAB-CBB
5	D	1311[A]	FEC	C2C-CAC-CBC-CGC
5	F	1507[A]	FEC	C2C-CAC-CBC-CGC
5	M	2207[B]	FEC	C2C-CAC-CBC-CGC
4	H	1710	GOL	O1-C1-C2-O2
4	I	1713	GOL	O2-C2-C3-O3
4	N	2310	GOL	O2-C2-C3-O3
4	O	2411	GOL	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	P	2510	GOL	O1-C1-C2-O2
4	B	1011	GOL	O1-C1-C2-O2
4	D	1211	GOL	O1-C1-C2-O2
4	D	1211	GOL	O2-C2-C3-O3
4	E	1411	GOL	O1-C1-C2-O2
4	E	1411	GOL	O2-C2-C3-O3
4	F	1510	GOL	O1-C1-C2-O2
4	G	1610	GOL	O2-C2-C3-O3
4	G	1611	GOL	O1-C1-C2-O2
4	H	1814	GOL	O1-C1-C2-O2
4	H	1814	GOL	O2-C2-C3-O3
4	J	1811	GOL	O1-C1-C2-O2
4	J	1811	GOL	O2-C2-C3-O3
4	O	2411	GOL	O1-C1-C2-O2
4	P	2510	GOL	O2-C2-C3-O3
5	F	1507[A]	FEC	C3D-CAD-CBD-CGD
5	G	1608[B]	FEC	C2C-CAC-CBC-CGC
5	M	2207[A]	FEC	C2C-CAC-CBC-CGC
4	A	1010	GOL	O2-C2-C3-O3
4	B	1110	GOL	O2-C2-C3-O3
4	E	1410	GOL	O2-C2-C3-O3
4	I	1713	GOL	O1-C1-C2-O2
4	I	1810	GOL	O2-C2-C3-O3
4	J	1910	GOL	O2-C2-C3-O3
4	K	2011	GOL	O1-C1-C2-O2
4	M	2210	GOL	O1-C1-C2-O2
4	M	2211	GOL	O1-C1-C2-O2
4	M	2211	GOL	O2-C2-C3-O3
4	O	2410	GOL	O2-C2-C3-O3
4	G	1610	GOL	O1-C1-C2-O2
4	M	2210	GOL	O2-C2-C3-O3
4	B	1011	GOL	O2-C2-C3-O3
4	B	1110	GOL	O1-C1-C2-O2
4	F	1510	GOL	O2-C2-C3-O3
4	F	1512	GOL	O1-C1-C2-O2
4	F	1512	GOL	O2-C2-C3-O3
4	N	2310	GOL	O1-C1-C2-O2
4	D	1211	GOL	C1-C2-C3-O3
4	G	1610	GOL	O1-C1-C2-C3
4	K	2011	GOL	C1-C2-C3-O3
5	I	1807[A]	FEC	C3D-CAD-CBD-CGD
5	G	1608[A]	FEC	C2C-CAC-CBC-CGC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	I	1807[A]	FEC	C2C-CAC-CBC-CGC
4	H	1710	GOL	O2-C2-C3-O3
5	M	2207[A]	FEC	C3D-CAD-CBD-CGD
5	M	2207[B]	FEC	C3D-CAD-CBD-CGD
5	I	1807[B]	FEC	CAD-CBD-CGD-O1D
5	P	2507[B]	FEC	CAD-CBD-CGD-O1D
5	I	1807[A]	FEC	CAA-CBA-CGA-O2A
5	B	1107[A]	FEC	CAA-CBA-CGA-O2A
5	M	2207[B]	FEC	CAC-CBC-CGC-O1C
5	P	2507[A]	FEC	CAA-CBA-CGA-O2A
5	D	1311[A]	FEC	C3D-CAD-CBD-CGD
5	G	1608[A]	FEC	C3D-CAD-CBD-CGD
5	L	2108[A]	FEC	C3D-CAD-CBD-CGD
5	L	2108[A]	FEC	CAA-CBA-CGA-O1A
5	M	2207[A]	FEC	CAA-CBA-CGA-O2A
5	B	1107[A]	FEC	CAC-CBC-CGC-O1C
5	D	1311[A]	FEC	CAA-CBA-CGA-O2A
5	L	2108[B]	FEC	CAD-CBD-CGD-O1D
5	F	1507[A]	FEC	CAA-CBA-CGA-O1A
5	G	1608[A]	FEC	CAA-CBA-CGA-O2A
5	L	2108[A]	FEC	CAA-CBA-CGA-O2A
5	F	1507[A]	FEC	CAA-CBA-CGA-O2A
5	G	1608[A]	FEC	CAA-CBA-CGA-O1A
5	P	2507[A]	FEC	CAA-CBA-CGA-O1A
5	B	1107[A]	FEC	CAA-CBA-CGA-O1A
5	B	1107[A]	FEC	CAC-CBC-CGC-O2C
5	F	1507[A]	FEC	CAC-CBC-CGC-O1C
5	M	2207[A]	FEC	CAA-CBA-CGA-O1A
5	M	2207[A]	FEC	CAC-CBC-CGC-O1C
5	B	1107[A]	FEC	C3D-CAD-CBD-CGD
5	B	1107[B]	FEC	C3D-CAD-CBD-CGD
5	G	1608[B]	FEC	CAA-CBA-CGA-O2A
5	I	1807[B]	FEC	CAA-CBA-CGA-O2A
5	I	1807[B]	FEC	CAD-CBD-CGD-O2D
5	P	2507[B]	FEC	CAD-CBD-CGD-O2D
5	D	1311[A]	FEC	CAA-CBA-CGA-O1A
5	M	2207[A]	FEC	CAC-CBC-CGC-O2C
5	L	2108[A]	FEC	CAC-CBC-CGC-O2C
5	L	2108[B]	FEC	CAC-CBC-CGC-O2C
5	D	1311[A]	FEC	CAC-CBC-CGC-O1C
5	L	2108[A]	FEC	CAC-CBC-CGC-O1C
5	M	2207[B]	FEC	CAC-CBC-CGC-O2C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	D	1311[A]	FEC	CAC-CBC-CGC-O2C
5	P	2507[A]	FEC	CAC-CBC-CGC-O2C
5	F	1507[B]	FEC	CAA-CBA-CGA-O1A
5	D	1311[B]	FEC	CAA-CBA-CGA-O1A
5	G	1608[B]	FEC	CAD-CBD-CGD-O1D
5	I	1807[A]	FEC	CAA-CBA-CGA-O1A
4	I	1713	GOL	C1-C2-C3-O3
4	I	1810	GOL	C1-C2-C3-O3
4	O	2411	GOL	O1-C1-C2-C3
5	I	1807[B]	FEC	C3D-CAD-CBD-CGD
5	G	1608[B]	FEC	CAA-CBA-CGA-O1A
5	I	1807[B]	FEC	CAA-CBA-CGA-O1A
5	G	1608[A]	FEC	CAC-CBC-CGC-O2C
5	B	1107[B]	FEC	CAA-CBA-CGA-O1A
5	F	1507[B]	FEC	CAA-CBA-CGA-O2A
5	L	2108[B]	FEC	CAC-CBC-CGC-O1C
5	P	2507[A]	FEC	CAC-CBC-CGC-O1C
5	I	1807[A]	FEC	CAC-CBC-CGC-O2C
5	I	1807[B]	FEC	CAC-CBC-CGC-O1C
5	F	1507[A]	FEC	CAC-CBC-CGC-O2C
5	I	1807[A]	FEC	CAC-CBC-CGC-O1C
5	I	1807[B]	FEC	CAC-CBC-CGC-O2C
5	L	2108[B]	FEC	CAA-CBA-CGA-O1A
5	D	1311[B]	FEC	CAC-CBC-CGC-O2C
5	G	1608[B]	FEC	CAC-CBC-CGC-O2C
5	P	2507[B]	FEC	CAA-CBA-CGA-O1A
5	D	1311[B]	FEC	CAD-CBD-CGD-O1D
5	I	1807[B]	FEC	CAB-CBB-CGB-O2B
5	I	1807[A]	FEC	CAD-CBD-CGD-O1D
5	L	2108[B]	FEC	CAD-CBD-CGD-O2D
5	L	2108[B]	FEC	C2C-CAC-CBC-CGC
5	M	2207[A]	FEC	CAD-CBD-CGD-O1D
5	P	2507[B]	FEC	CAB-CBB-CGB-O2B
5	B	1107[B]	FEC	CAA-CBA-CGA-O2A
5	D	1311[B]	FEC	CAA-CBA-CGA-O2A
5	L	2108[B]	FEC	CAA-CBA-CGA-O2A
5	I	1807[A]	FEC	CAD-CBD-CGD-O2D
5	D	1311[A]	FEC	CAD-CBD-CGD-O1D
5	D	1311[B]	FEC	CAC-CBC-CGC-O1C
5	L	2108[A]	FEC	CAD-CBD-CGD-O1D
5	P	2507[B]	FEC	CAB-CBB-CGB-O1B
5	G	1608[A]	FEC	CAC-CBC-CGC-O1C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	I	1807[B]	FEC	CAB-CBB-CGB-O1B
5	M	2207[A]	FEC	CAD-CBD-CGD-O2D
5	B	1107[A]	FEC	CAD-CBD-CGD-O1D
5	P	2507[B]	FEC	CAA-CBA-CGA-O2A
5	D	1311[A]	FEC	CAD-CBD-CGD-O2D
5	D	1311[B]	FEC	CAD-CBD-CGD-O2D
5	G	1608[B]	FEC	CAC-CBC-CGC-O1C
5	G	1608[B]	FEC	CAD-CBD-CGD-O2D
4	C	1210	GOL	C1-C2-C3-O3
4	E	1411	GOL	C1-C2-C3-O3
5	P	2507[A]	FEC	CAD-CBD-CGD-O2D
5	B	1107[A]	FEC	CAD-CBD-CGD-O2D
5	B	1107[B]	FEC	C2B-C3B-CAB-CBB
5	F	1507[B]	FEC	CAC-CBC-CGC-O2C
5	L	2108[A]	FEC	CAD-CBD-CGD-O2D
5	P	2507[A]	FEC	CAD-CBD-CGD-O1D
5	B	1107[B]	FEC	CAB-CBB-CGB-O2B
5	M	2207[B]	FEC	CAD-CBD-CGD-O1D
5	F	1507[B]	FEC	CAD-CBD-CGD-O1D
5	G	1608[A]	FEC	CAD-CBD-CGD-O1D
5	G	1608[A]	FEC	CAD-CBD-CGD-O2D
5	M	2207[B]	FEC	CAD-CBD-CGD-O2D
5	B	1107[B]	FEC	CAB-CBB-CGB-O1B

There are no ring outliers.

59 monomers are involved in 247 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	2011	GOL	1	0
3	P	2506	SO4	1	0
4	G	1611	GOL	1	0
3	P	2501	SO4	1	0
4	I	1810	GOL	15	0
3	M	2206	SO4	2	0
5	I	1807[B]	FEC	9	0
3	L	2102	SO4	1	7
4	J	1811	GOL	1	0
5	L	2108[B]	FEC	12	0
5	P	2507[A]	FEC	8	0
3	K	1504	SO4	1	0
4	B	1110	GOL	3	0
4	M	2211	GOL	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	P	2510	GOL	2	0
5	D	1311[A]	FEC	8	0
5	M	2207[B]	FEC	8	0
3	B	1005	SO4	1	0
4	D	1211	GOL	5	0
4	I	1713	GOL	1	0
3	B	1106	SO4	1	0
4	M	2210	GOL	5	0
4	H	1710	GOL	1	0
3	L	2107	SO4	1	0
3	O	2406	SO4	1	0
4	E	1410	GOL	6	0
4	J	1910	GOL	4	0
5	L	2108[A]	FEC	11	0
4	O	2411	GOL	2	0
3	F	1502	SO4	2	0
5	F	1507[B]	FEC	13	0
3	A	1105	SO4	3	0
6	D	1310	3PY	1	0
3	F	1501	SO4	1	0
3	B	1104	SO4	1	0
3	O	2409	SO4	1	0
5	G	1608[B]	FEC	6	0
4	F	1510	GOL	3	0
3	C	1206	SO4	1	0
3	J	1904	SO4	1	0
5	F	1507[A]	FEC	4	0
5	I	1807[A]	FEC	9	0
3	G	1606	SO4	1	0
3	E	1304	SO4	1	0
3	L	2103	SO4	1	0
3	J	1906	SO4	3	0
5	B	1107[B]	FEC	7	0
3	I	1803	SO4	1	0
5	M	2207[A]	FEC	10	0
3	C	1203	SO4	1	0
5	G	1608[A]	FEC	9	0
4	G	1610	GOL	2	0
4	N	2310	GOL	1	0
3	I	1802	SO4	1	7
4	O	2410	GOL	2	0
5	P	2507[B]	FEC	13	0

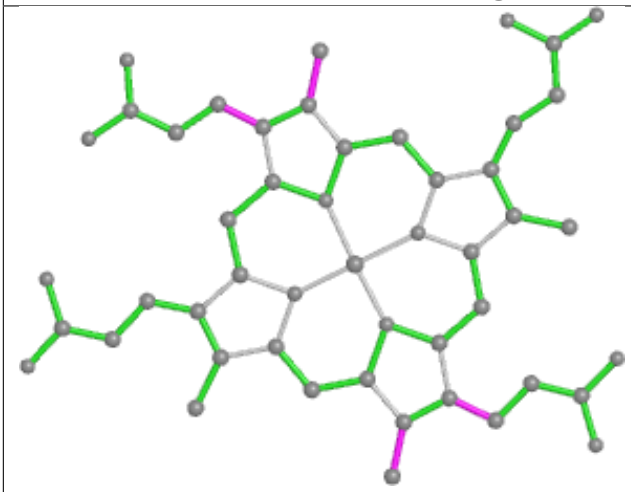
Continued on next page...

Continued from previous page...

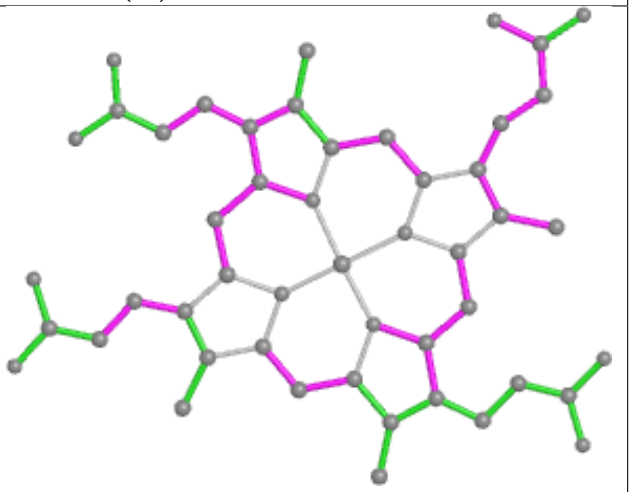
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1107[A]	FEC	10	0
4	A	1010	GOL	1	0
5	D	1311[B]	FEC	14	0

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.

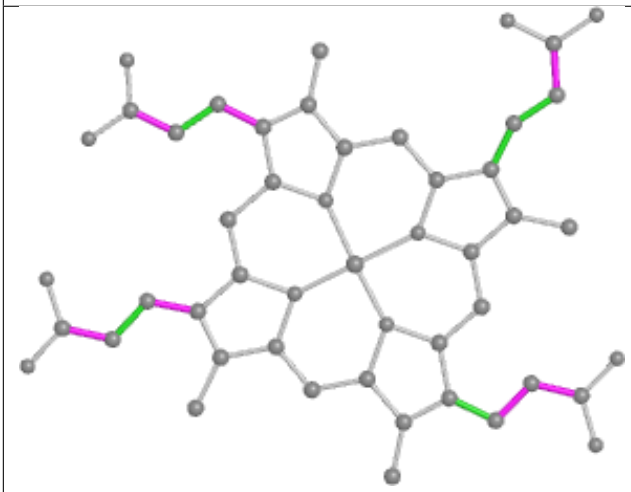
Ligand FEC I 1807 (B)



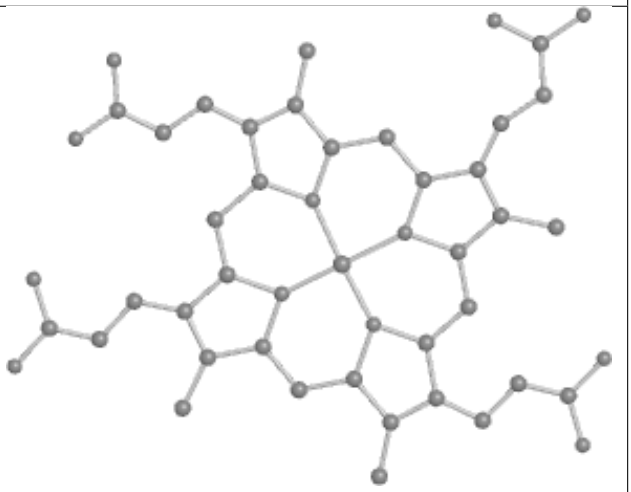
Bond lengths



Bond angles

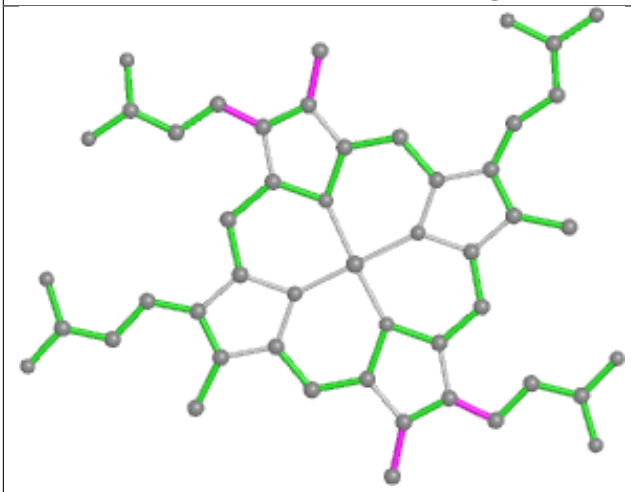


Torsions

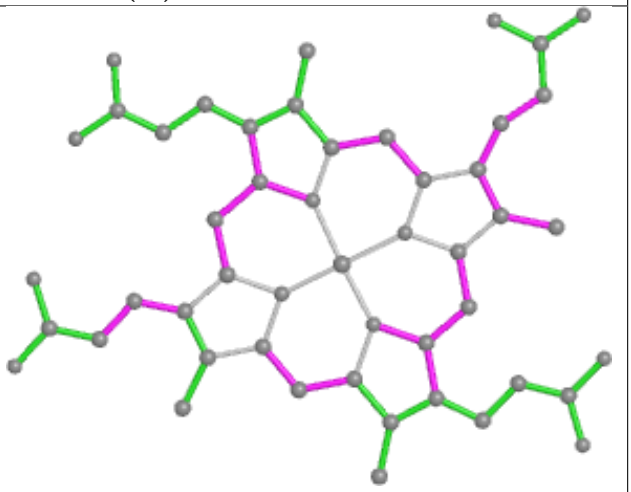


Rings

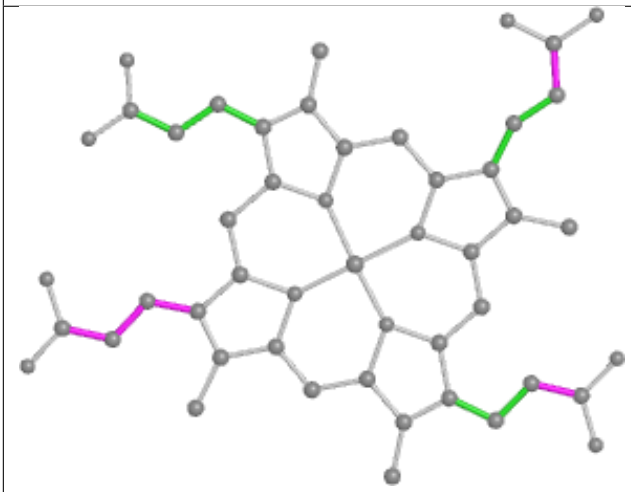
Ligand FEC L 2108 (B)



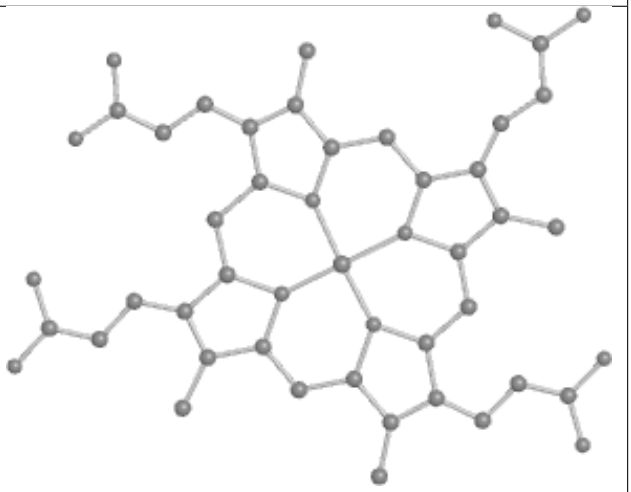
Bond lengths



Bond angles

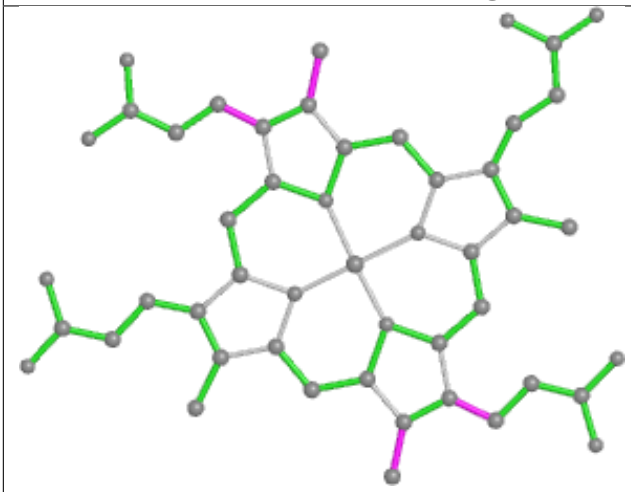


Torsions

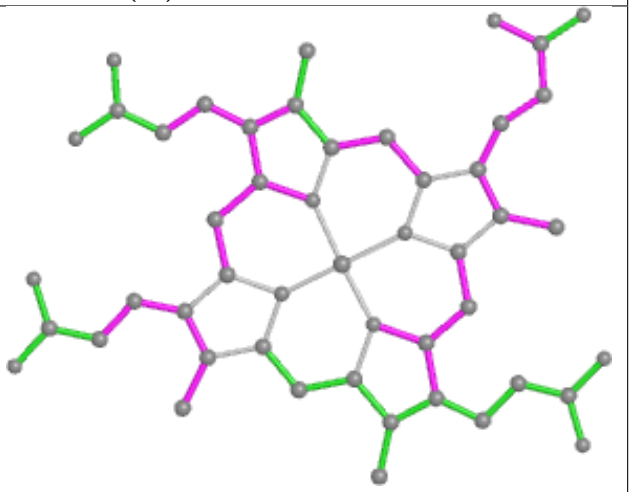


Rings

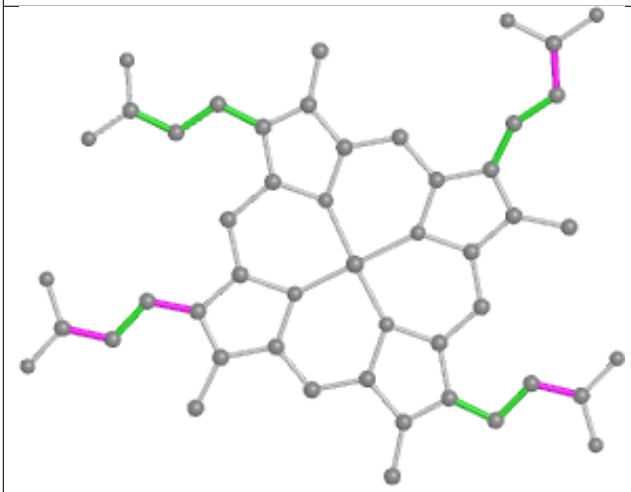
Ligand FEC P 2507 (A)



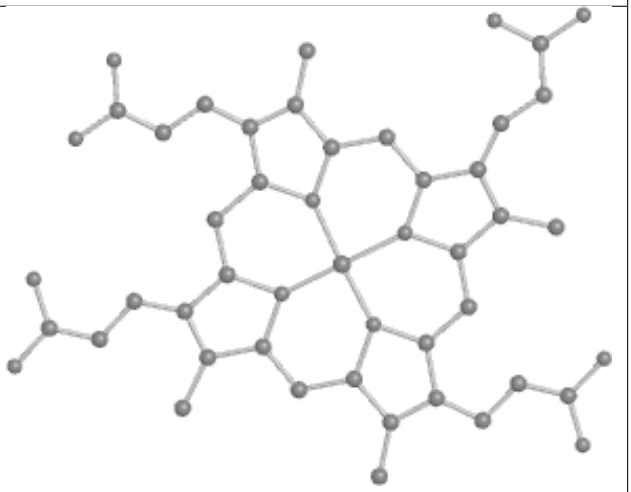
Bond lengths



Bond angles

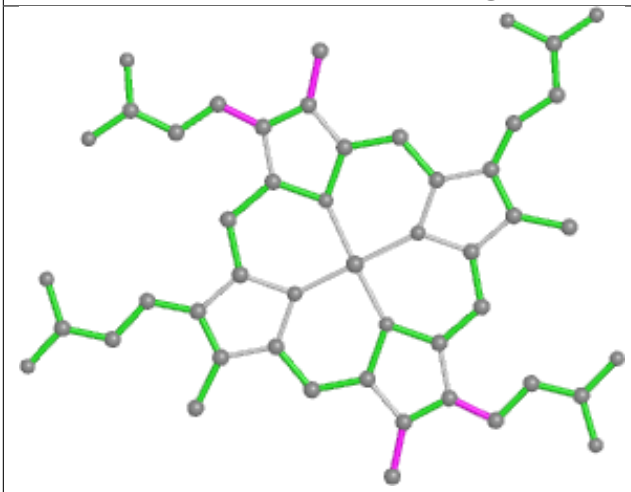


Torsions

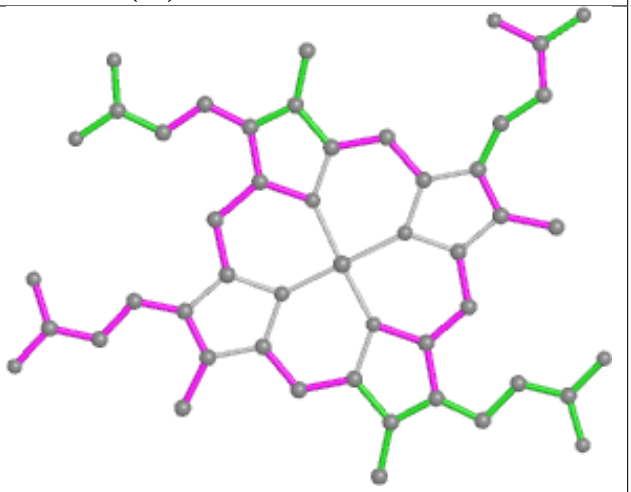


Rings

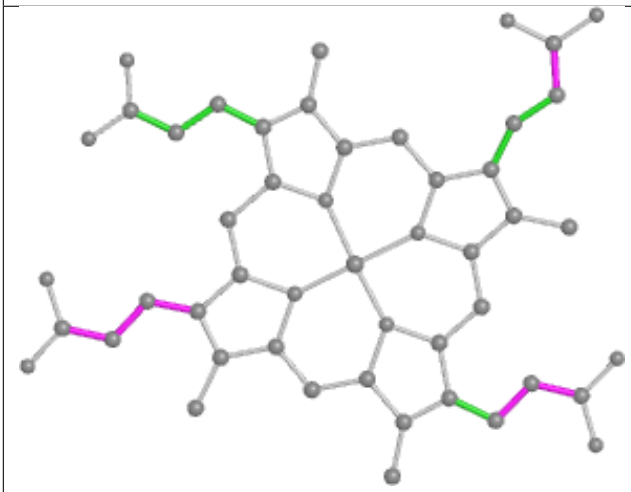
Ligand FEC D 1311 (A)



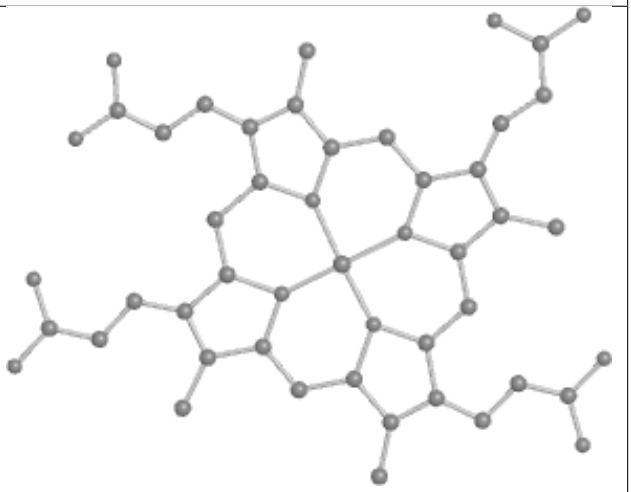
Bond lengths



Bond angles

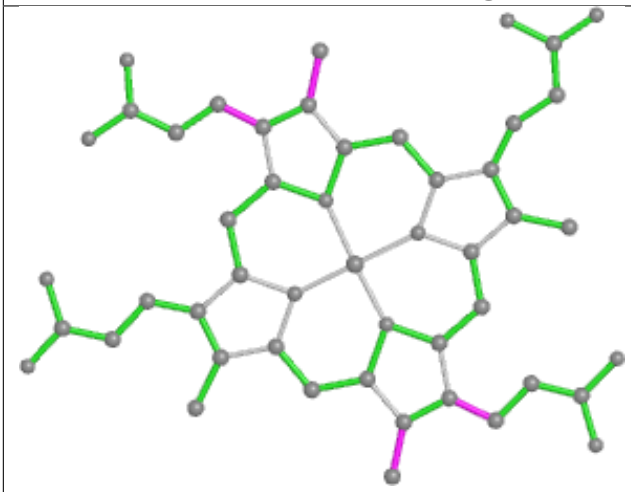


Torsions

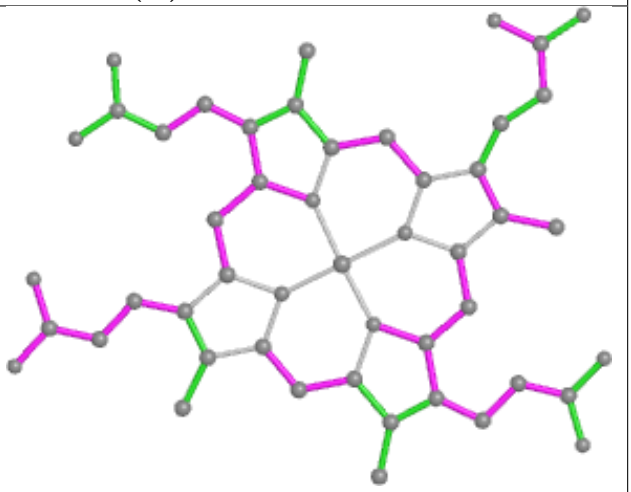


Rings

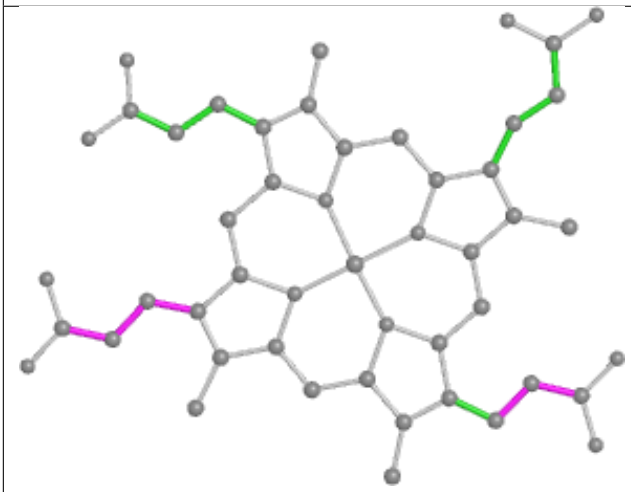
Ligand FEC M 2207 (B)



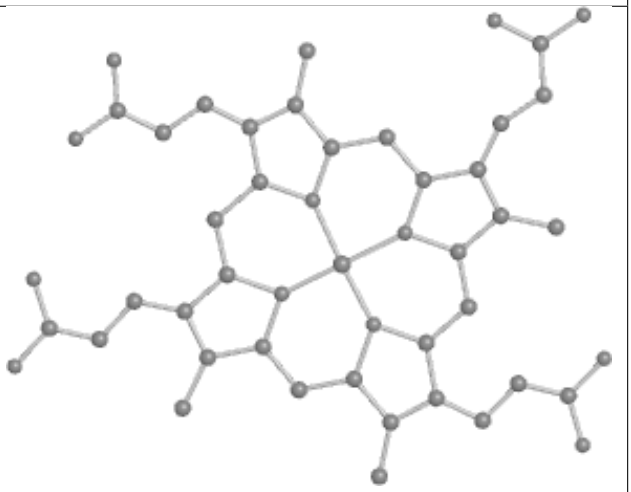
Bond lengths



Bond angles

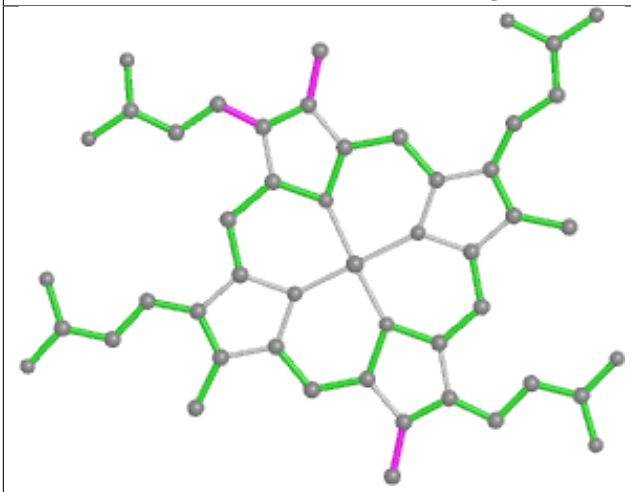


Torsions

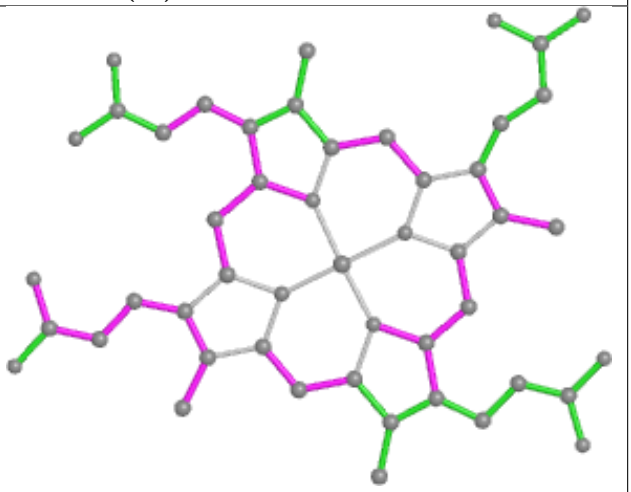


Rings

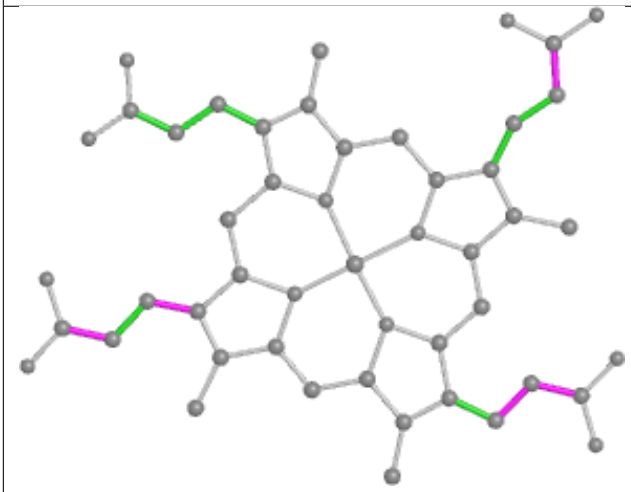
Ligand FEC L 2108 (A)



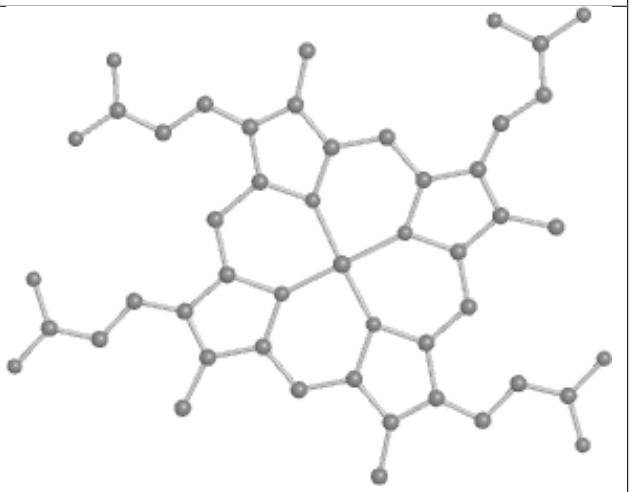
Bond lengths



Bond angles

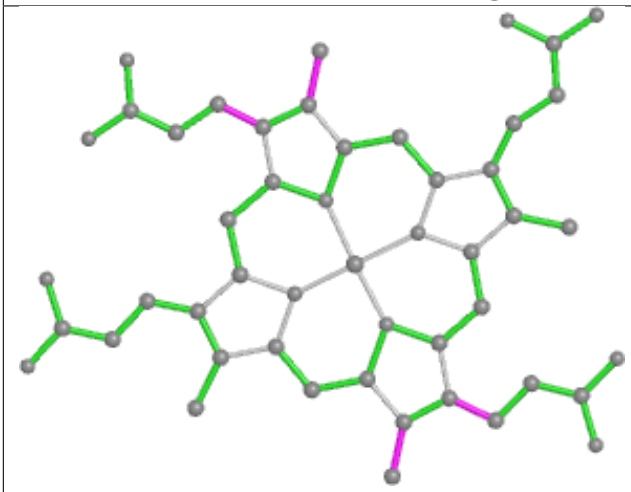


Torsions

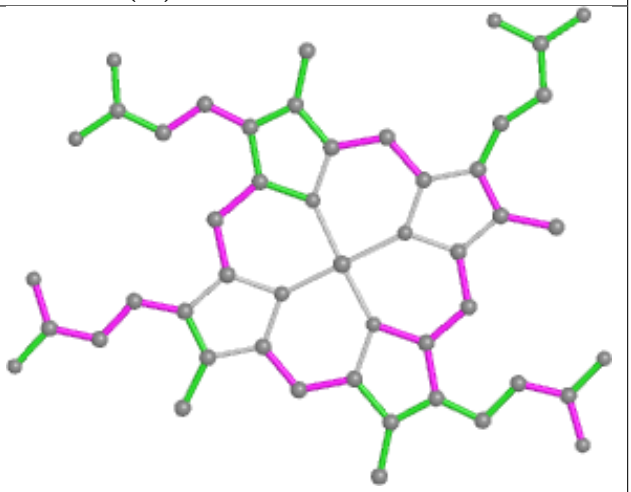


Rings

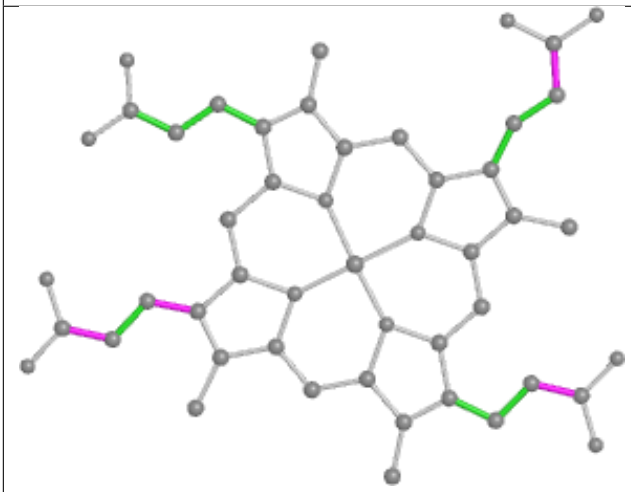
Ligand FEC F 1507 (B)



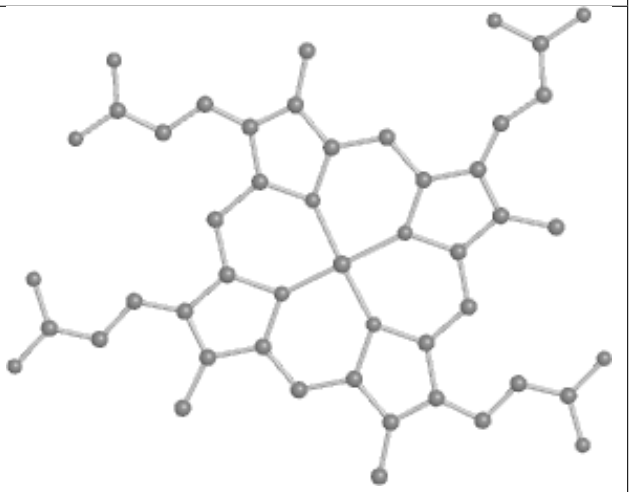
Bond lengths



Bond angles

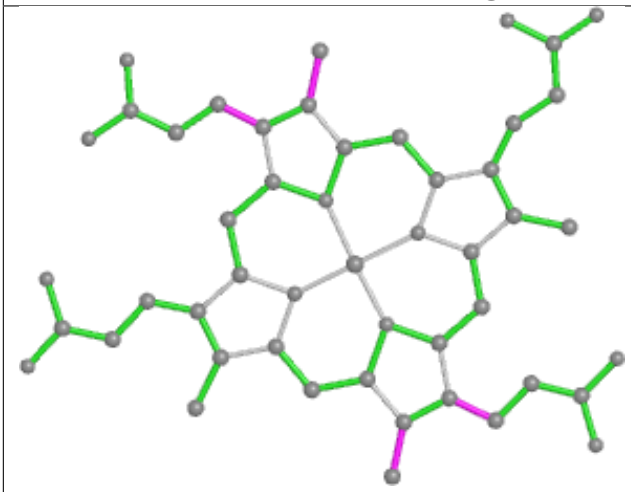


Torsions

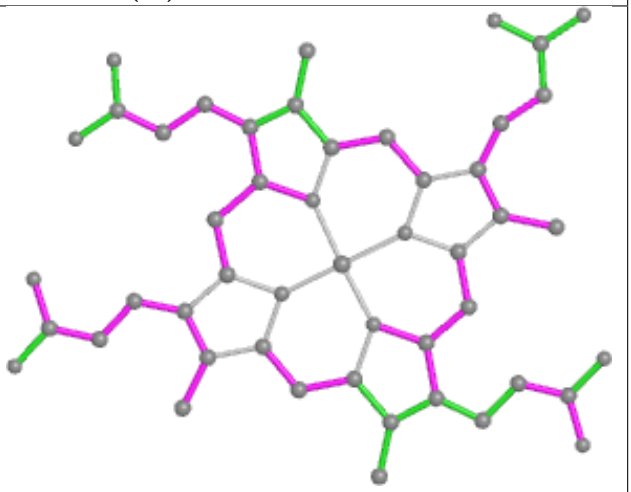


Rings

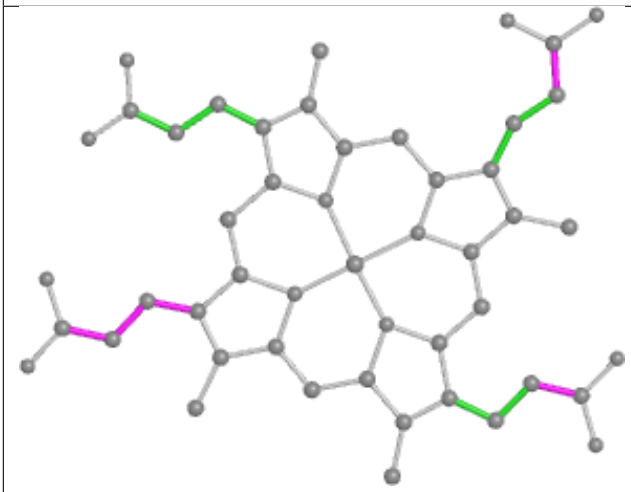
Ligand FEC G 1608 (B)



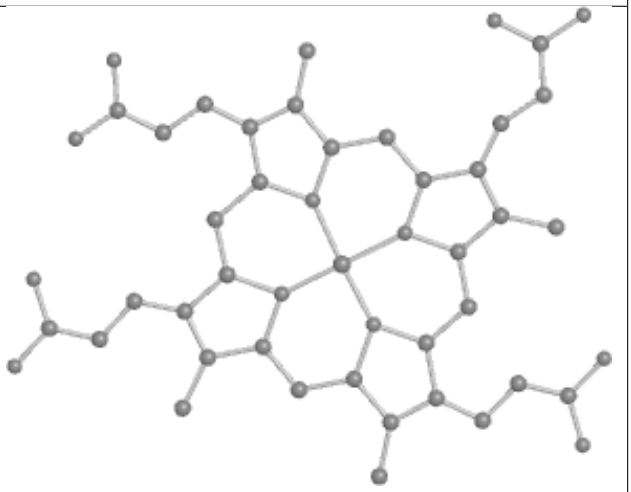
Bond lengths



Bond angles

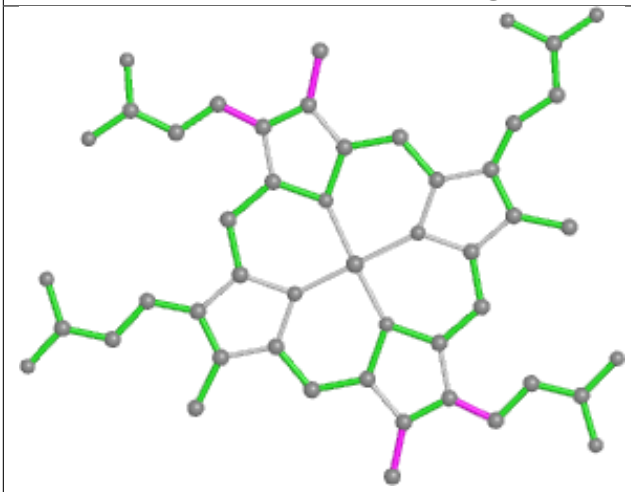


Torsions

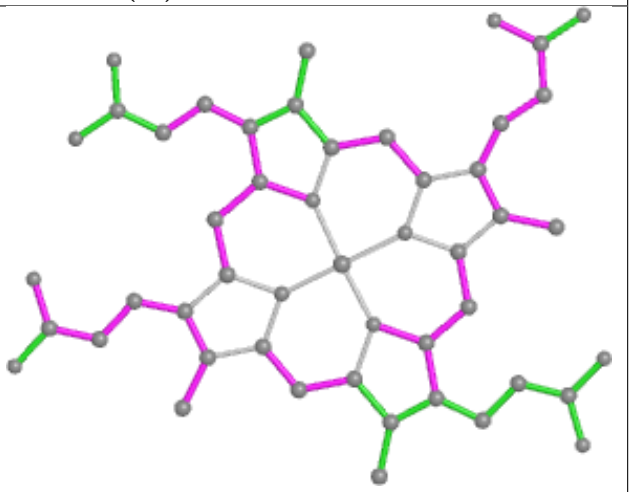


Rings

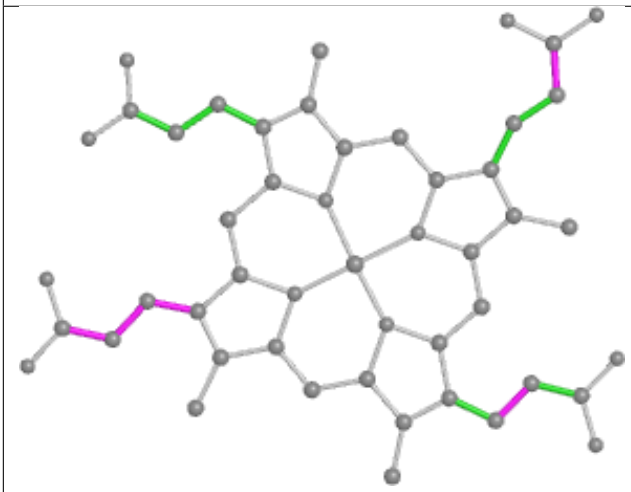
Ligand FEC F 1507 (A)



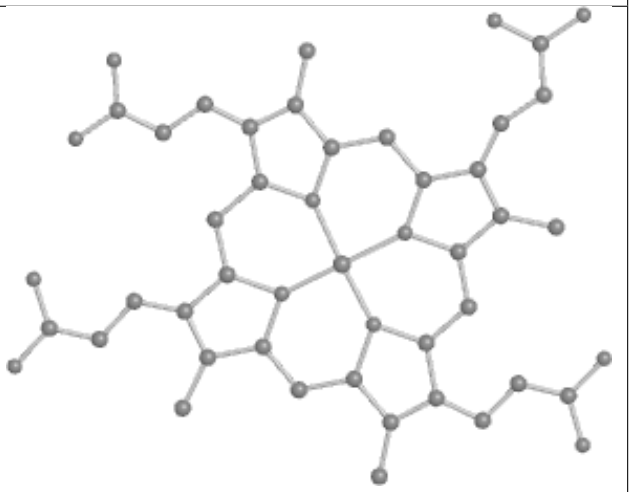
Bond lengths



Bond angles

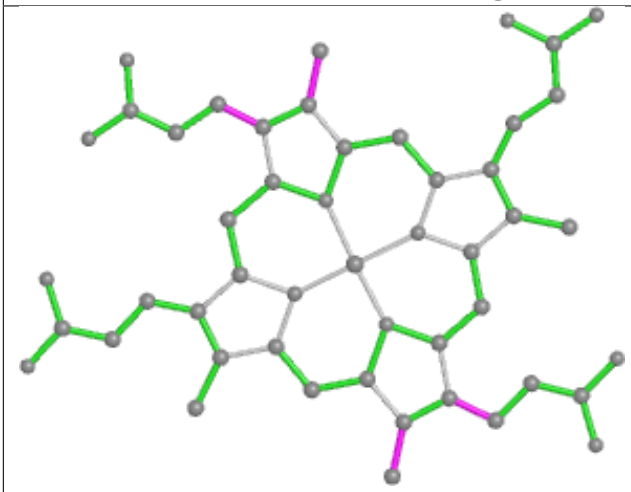


Torsions

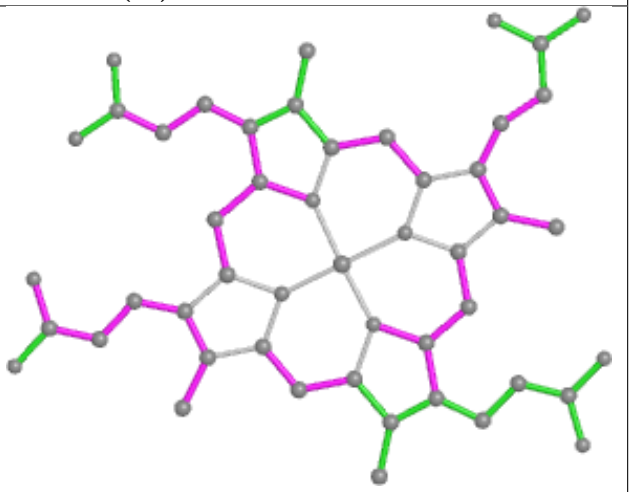


Rings

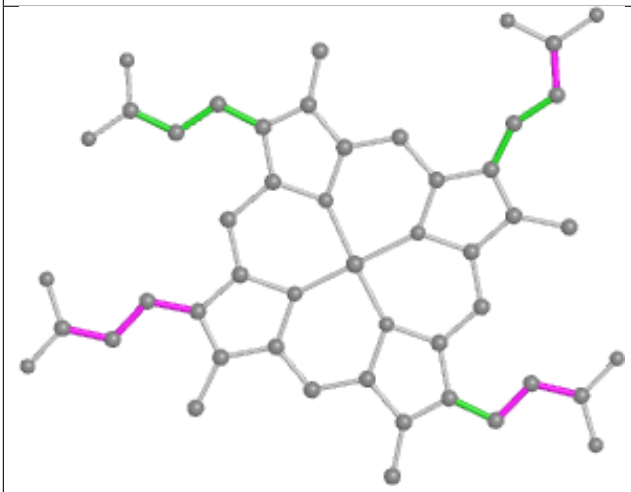
Ligand FEC I 1807 (A)



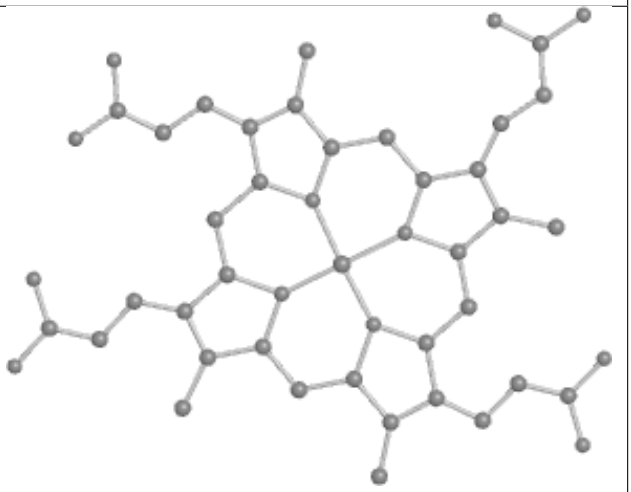
Bond lengths



Bond angles

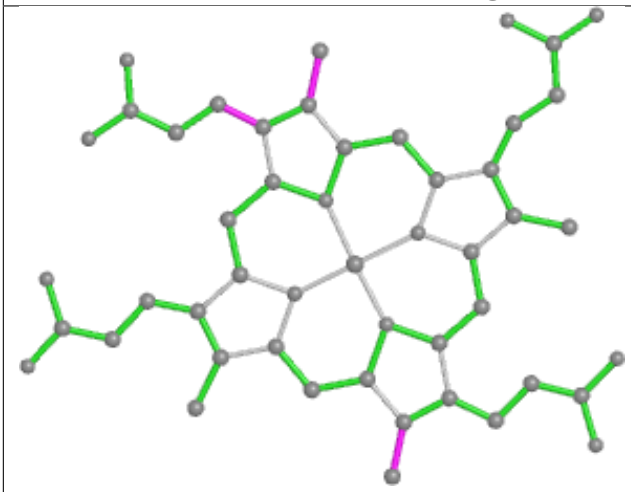


Torsions

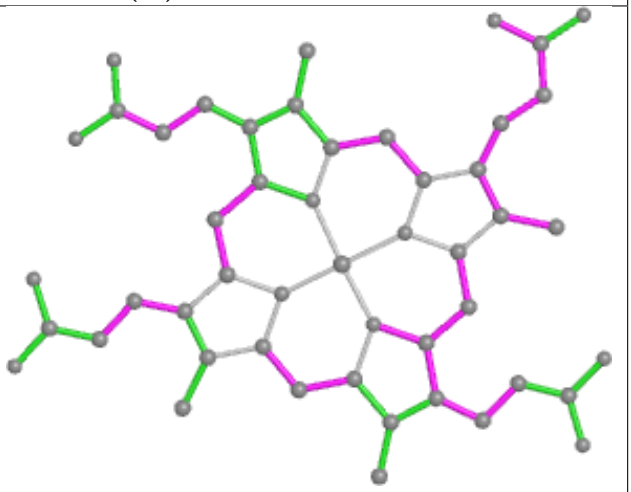


Rings

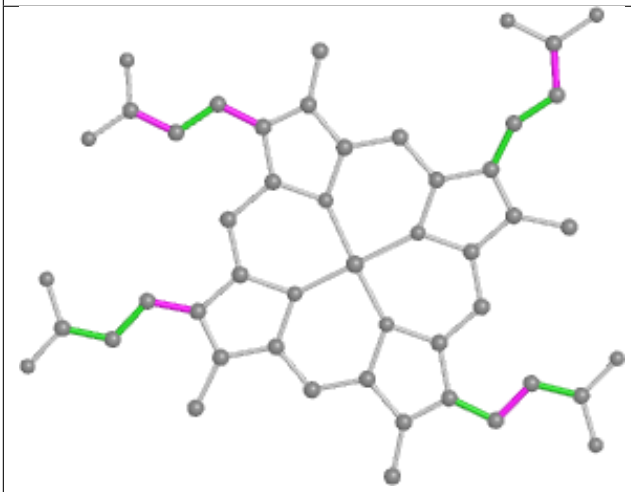
Ligand FEC B 1107 (B)



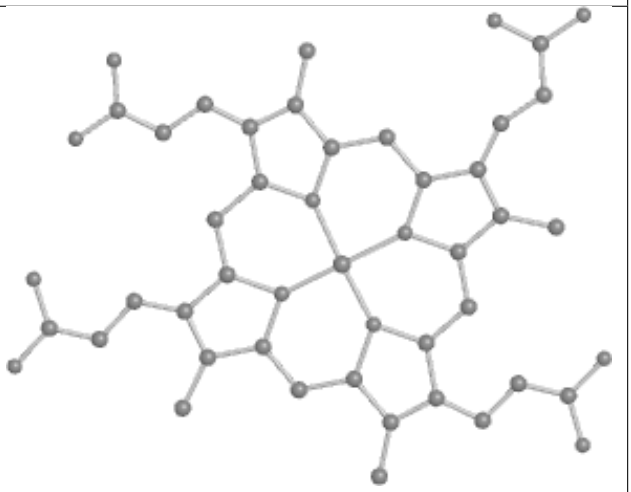
Bond lengths



Bond angles

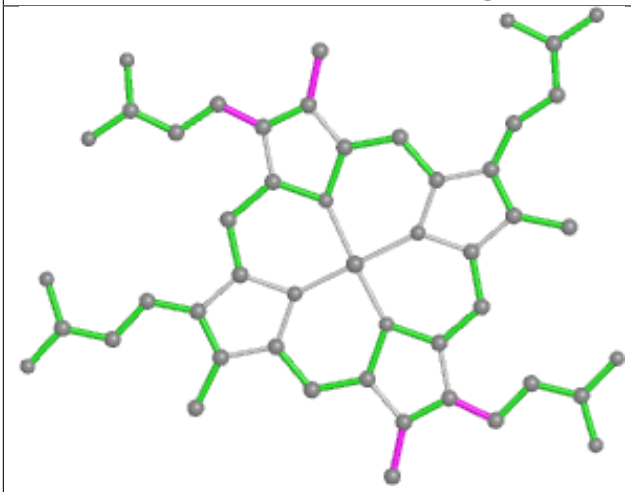


Torsions

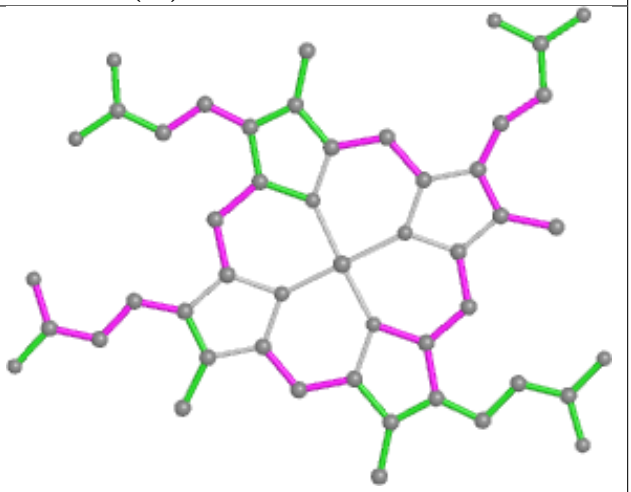


Rings

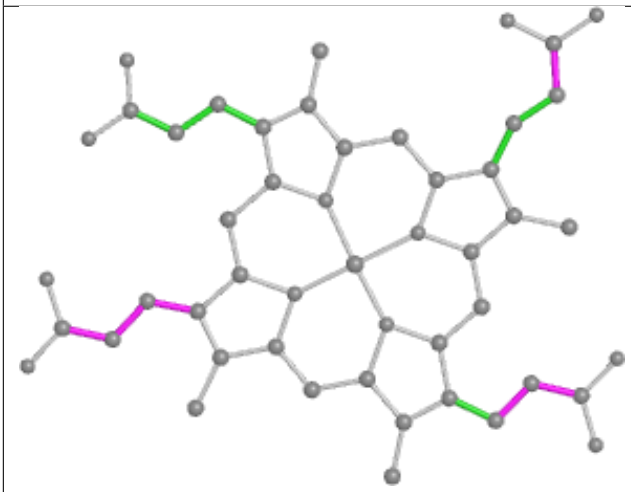
Ligand FEC M 2207 (A)



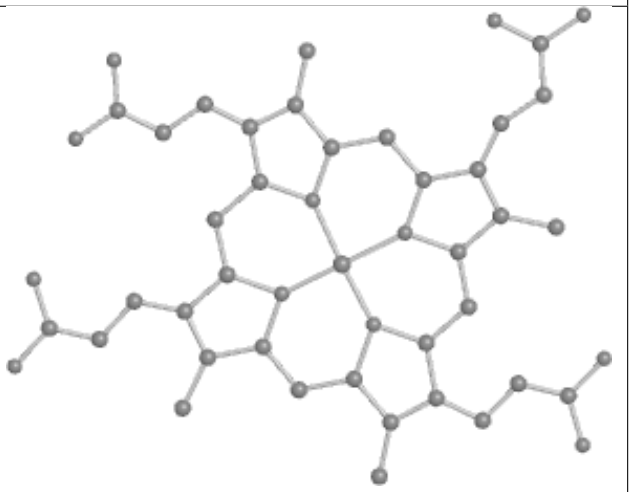
Bond lengths



Bond angles

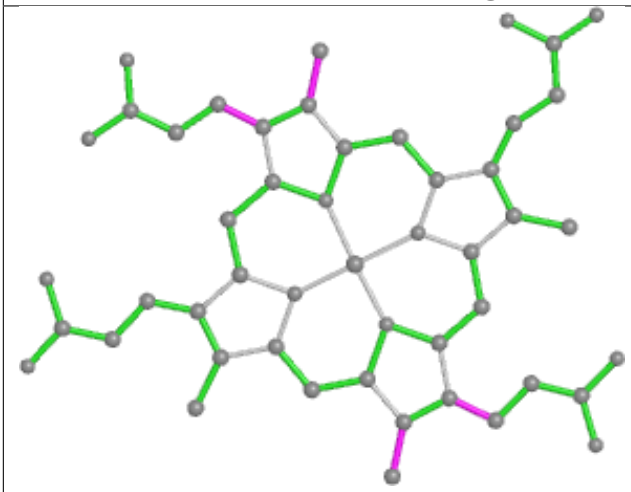


Torsions

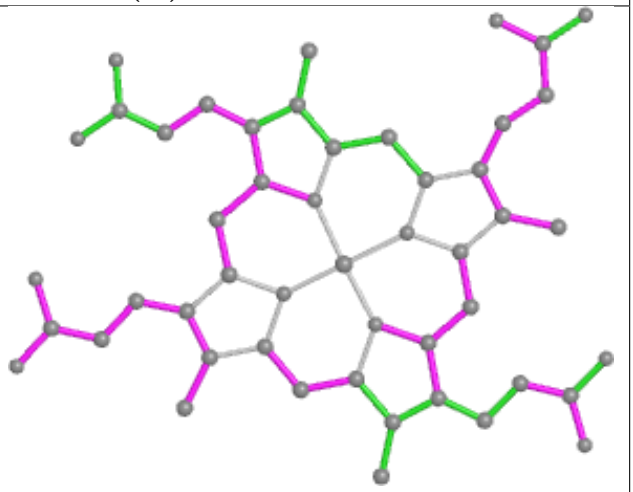


Rings

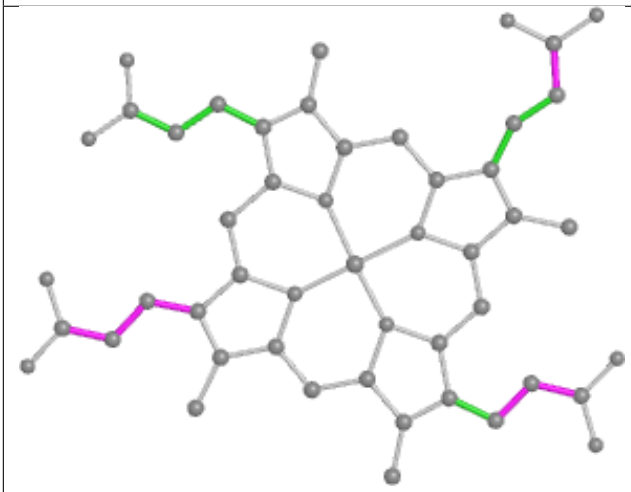
Ligand FEC G 1608 (A)



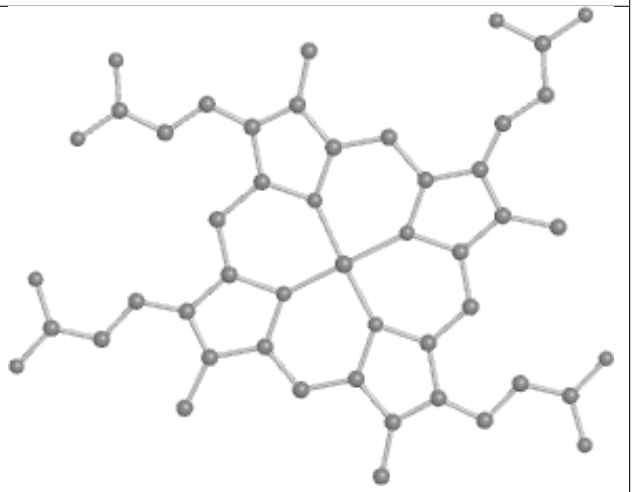
Bond lengths



Bond angles

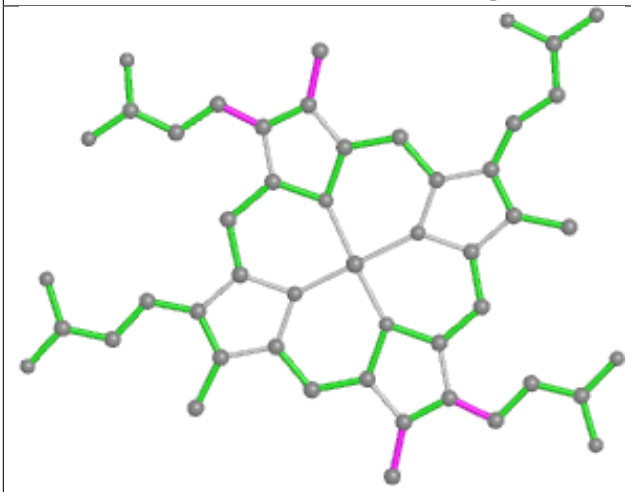


Torsions

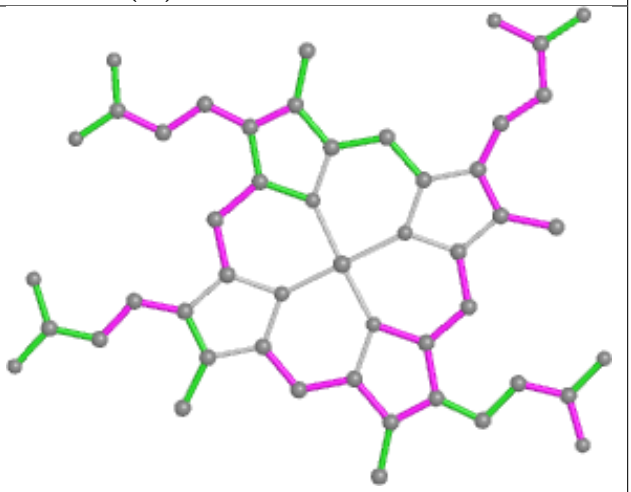


Rings

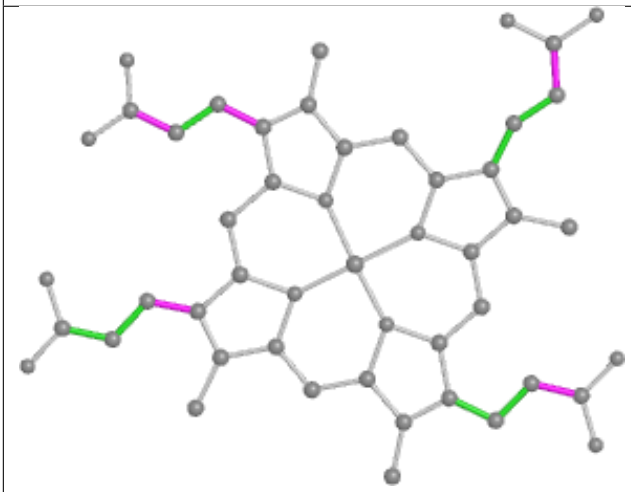
Ligand FEC P 2507 (B)



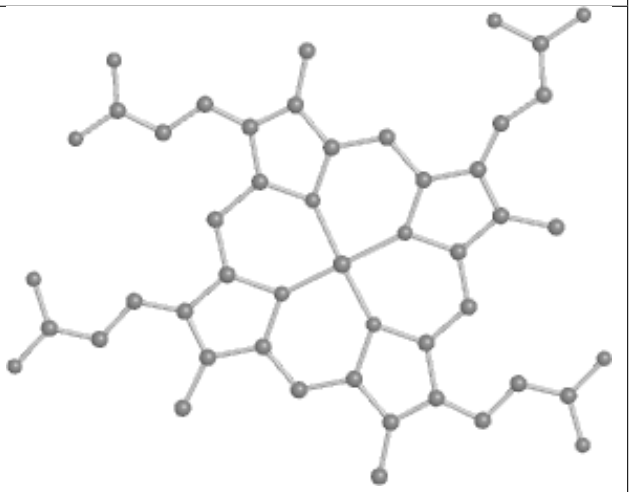
Bond lengths



Bond angles

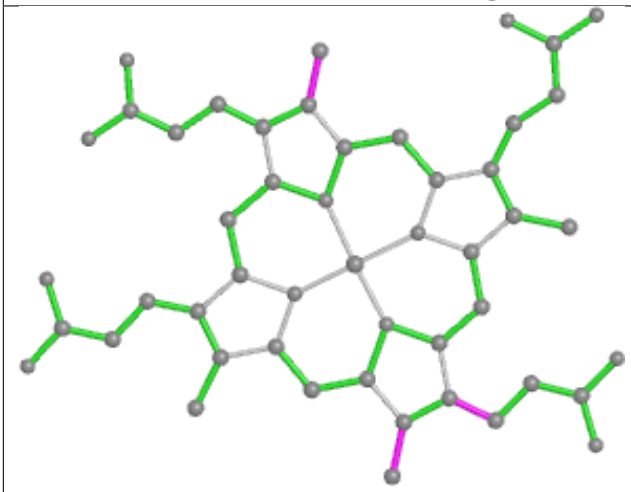


Torsions

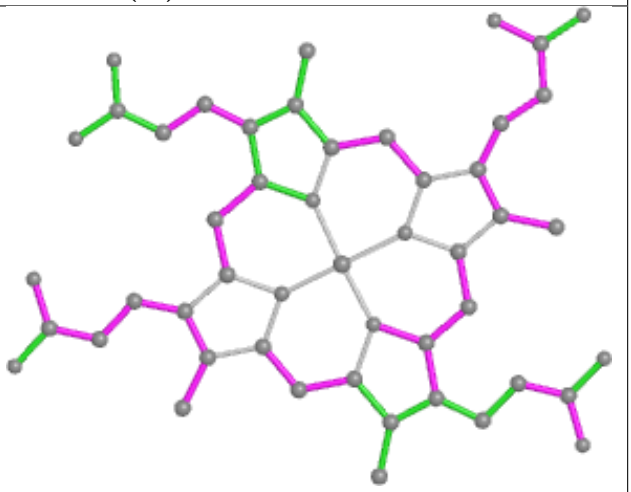


Rings

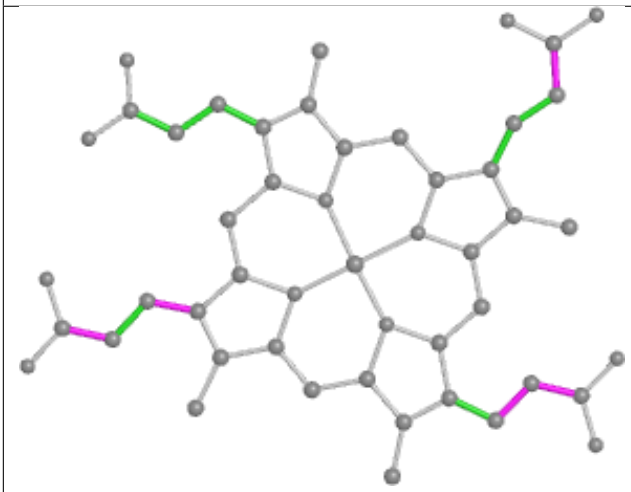
Ligand FEC B 1107 (A)



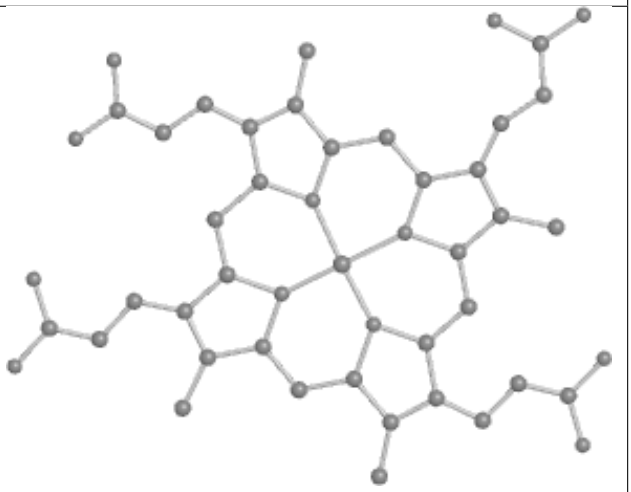
Bond lengths



Bond angles

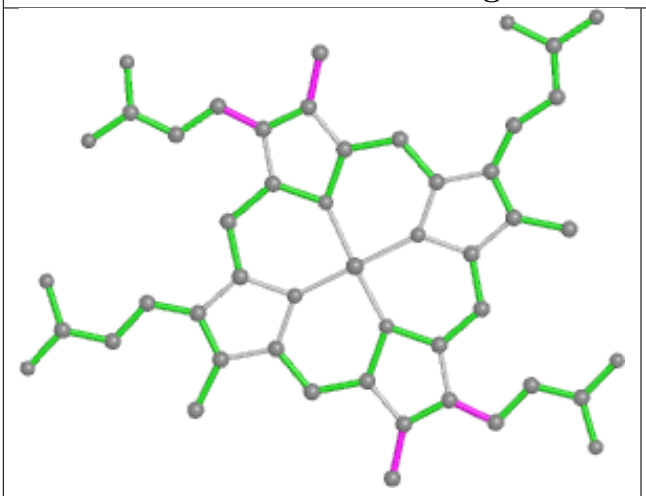


Torsions

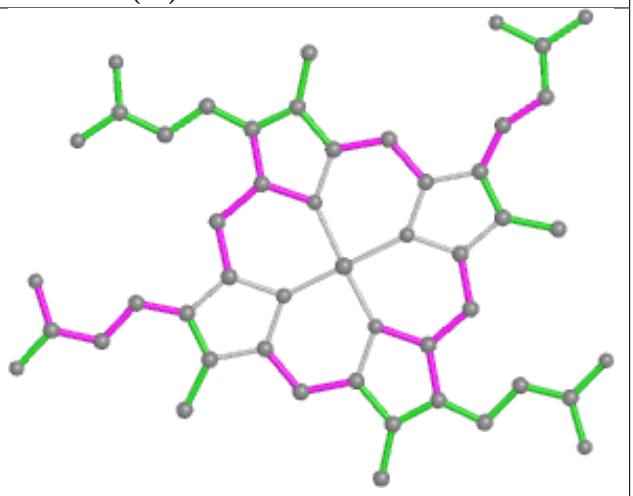


Rings

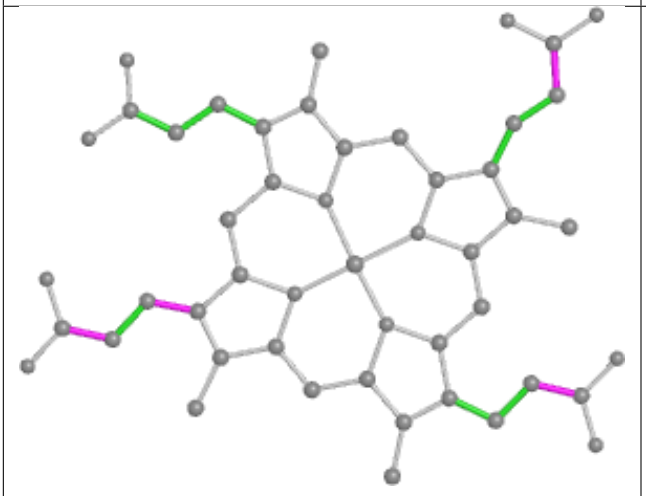
Ligand FEC D 1311 (B)



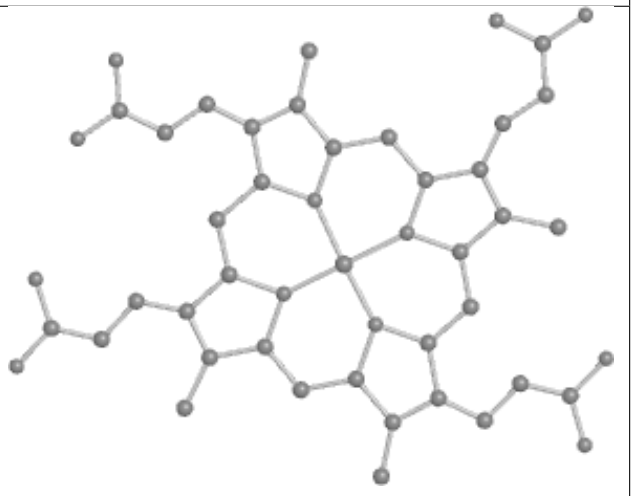
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	169/179 (94%)	0.11	10 (5%)	22	30	16, 24, 43, 65	0
1	B	170/179 (94%)	-0.03	9 (5%)	26	35	15, 24, 45, 65	0
1	C	170/179 (94%)	-0.05	8 (4%)	31	41	16, 25, 45, 65	0
1	D	170/179 (94%)	0.02	9 (5%)	26	35	16, 25, 44, 65	1 (0%)
1	E	170/179 (94%)	0.05	9 (5%)	26	35	17, 25, 47, 65	1 (0%)
1	F	170/179 (94%)	-0.03	7 (4%)	37	46	16, 25, 46, 68	1 (0%)
1	G	169/179 (94%)	-0.08	4 (2%)	59	68	15, 24, 43, 65	0
1	H	170/179 (94%)	0.01	12 (7%)	16	24	16, 25, 44, 65	0
1	I	170/179 (94%)	-0.00	6 (3%)	44	53	16, 24, 43, 65	0
1	J	170/179 (94%)	-0.02	9 (5%)	26	35	17, 25, 47, 65	0
1	K	170/179 (94%)	-0.06	4 (2%)	59	68	16, 24, 46, 68	0
1	L	170/179 (94%)	-0.01	4 (2%)	59	68	16, 24, 43, 65	1 (0%)
1	M	170/179 (94%)	-0.04	7 (4%)	37	46	15, 24, 47, 65	0
1	N	170/179 (94%)	-0.03	6 (3%)	44	53	16, 24, 43, 65	0
1	O	169/179 (94%)	0.10	6 (3%)	42	52	16, 25, 44, 68	1 (0%)
1	P	170/179 (94%)	-0.09	7 (4%)	37	46	17, 25, 48, 65	0
All	All	2717/2864 (94%)	-0.01	117 (4%)	35	45	15, 25, 46, 68	5 (0%)

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	166	THR	7.2
1	A	166	THR	7.1
1	E	168[A]	SER	6.8
1	N	166	THR	6.6
1	I	166	THR	6.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	168[A]	SER	6.3
1	O	166	THR	6.2
1	B	166	THR	6.0
1	I	168[A]	SER	5.8
1	L	166	THR	5.8
1	P	168[A]	SER	5.4
1	N	168[A]	SER	5.3
1	F	166	THR	5.2
1	E	166	THR	5.2
1	M	166	THR	4.9
1	A	168[A]	SER	4.9
1	D	168[A]	SER	4.8
1	K	168[A]	SER	4.7
1	L	168[A]	SER	4.7
1	M	168[A]	SER	4.6
1	F	168[A]	SER	4.6
1	J	168[A]	SER	4.5
1	H	166	THR	4.3
1	F	165	GLY	4.3
1	A	167	ALA	4.2
1	B	168[A]	SER	4.2
1	C	3	GLY	4.1
1	O	4	ASN	4.1
1	M	167	ALA	4.1
1	H	168[A]	SER	4.0
1	O	168[A]	SER	4.0
1	G	167	ALA	4.0
1	J	4	ASN	3.9
1	N	167	ALA	3.9
1	P	166	THR	3.8
1	C	168[A]	SER	3.7
1	F	3	GLY	3.6
1	J	166	THR	3.6
1	K	166	THR	3.6
1	C	165	GLY	3.4
1	A	27	ILE	3.4
1	D	166	THR	3.4
1	J	3	GLY	3.3
1	A	165	GLY	3.3
1	P	3	GLY	3.3
1	G	166	THR	3.3
1	I	169[A]	LYS	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	P	7	ASP	3.3
1	C	4	ASN	3.2
1	D	3	GLY	3.2
1	F	7	ASP	3.2
1	H	4	ASN	3.1
1	O	167	ALA	3.1
1	M	6	GLU	3.0
1	B	4	ASN	3.0
1	D	4	ASN	3.0
1	E	167	ALA	2.9
1	M	3	GLY	2.9
1	C	7	ASP	2.9
1	L	60	ALA	2.9
1	D	165	GLY	2.8
1	M	169[A]	LYS	2.8
1	J	169[A]	LYS	2.7
1	D	7	ASP	2.7
1	C	27	ILE	2.7
1	E	165	GLY	2.7
1	L	167	ALA	2.7
1	G	169[A]	LYS	2.6
1	D	5	ARG	2.6
1	M	4	ASN	2.6
1	H	27	ILE	2.6
1	E	6	GLU	2.6
1	O	165	GLY	2.6
1	F	167	ALA	2.5
1	J	7	ASP	2.5
1	I	3	GLY	2.5
1	H	3	GLY	2.5
1	E	7	ASP	2.5
1	C	167	ALA	2.5
1	A	127[A]	ARG	2.5
1	N	165	GLY	2.5
1	E	77	GLN	2.5
1	B	169[A]	LYS	2.5
1	N	3	GLY	2.4
1	H	169[A]	LYS	2.4
1	A	169[A]	LYS	2.4
1	H	167	ALA	2.4
1	H	165	GLY	2.4
1	B	7	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	81	LYS	2.3
1	I	167	ALA	2.3
1	E	27	ILE	2.3
1	K	169[A]	LYS	2.3
1	P	6	GLU	2.3
1	H	108	GLN	2.3
1	O	90	VAL	2.3
1	D	169[A]	LYS	2.3
1	P	79	GLU	2.2
1	H	24	LEU	2.2
1	B	167	ALA	2.2
1	E	4	ASN	2.2
1	J	81	LYS	2.2
1	B	165	GLY	2.2
1	J	5	ARG	2.2
1	K	27	ILE	2.2
1	P	167	ALA	2.2
1	A	4	ASN	2.1
1	I	27	ILE	2.1
1	J	165	GLY	2.1
1	F	4	ASN	2.1
1	B	27	ILE	2.1
1	H	7	ASP	2.1
1	B	3	GLY	2.1
1	A	24	LEU	2.0
1	A	31	MET	2.0
1	D	77[A]	GLN	2.0
1	N	6	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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
3	SO4	A	1004	5/5	0.45	0.48	66,66,67,67	5
3	SO4	G	1607	5/5	0.61	0.38	67,67,70,70	0
3	SO4	J	1901	5/5	0.73	0.29	66,67,67,69	0
3	SO4	K	1504	5/5	0.73	0.23	78,78,78,79	0
3	SO4	E	1304	5/5	0.75	0.39	65,65,67,67	0
3	SO4	O	2409	5/5	0.76	0.40	57,63,66,67	0
4	GOL	E	1411	6/6	0.77	0.19	34,56,92,108	0
2	FE	B	201	1/1	0.78	0.09	44,44,44,44	0
3	SO4	D	1303	5/5	0.78	0.23	39,44,45,50	5
4	GOL	J	1910	6/6	0.78	0.30	46,52,80,104	0
3	SO4	G	1603	5/5	0.79	0.41	73,73,74,75	0
3	SO4	P	2503	5/5	0.79	0.28	42,43,47,49	5
2	FE	L	201	1/1	0.79	0.11	42,42,42,42	0
4	GOL	I	1713	6/6	0.79	0.21	52,57,84,157	0
3	SO4	L	2103	5/5	0.79	0.36	78,78,78,79	0
3	SO4	H	1703	5/5	0.80	0.48	40,43,48,48	0
4	GOL	A	1010	6/6	0.81	0.29	42,68,89,111	0
4	GOL	I	1810	6/6	0.81	0.30	27,42,66,76	0
3	SO4	F	1502	5/5	0.81	0.44	69,69,69,71	0
3	SO4	K	2001	5/5	0.82	0.26	51,53,53,54	0
4	GOL	B	1110	6/6	0.82	0.20	40,46,69,84	0
4	GOL	H	1710	6/6	0.83	0.26	50,52,61,94	0
4	GOL	H	1814	6/6	0.83	0.16	38,49,55,61	0
3	SO4	E	1401	5/5	0.83	0.28	67,68,68,68	0
3	SO4	L	2101	5/5	0.83	0.20	64,64,65,65	0
4	GOL	G	1611	6/6	0.83	0.19	31,53,70,78	0
3	SO4	C	1201	5/5	0.84	0.19	65,65,67,67	0
3	SO4	P	2501	5/5	0.84	0.18	62,62,63,63	0
3	SO4	J	1906	5/5	0.85	0.35	50,51,59,59	0
3	SO4	M	2206	5/5	0.85	0.31	58,60,67,70	0
3	SO4	G	1606	5/5	0.86	0.26	58,65,67,73	0
4	GOL	G	1610	6/6	0.86	0.20	44,46,56,106	0
4	GOL	M	2211	6/6	0.86	0.16	40,61,98,143	0
4	GOL	P	2510	6/6	0.86	0.28	32,51,74,105	0
2	FE	M	201	1/1	0.87	0.10	40,40,40,40	0
4	GOL	C	1210	6/6	0.87	0.29	32,43,67,71	0
3	SO4	C	1206	5/5	0.87	0.36	46,46,47,49	0
3	SO4	D	1301	5/5	0.87	0.24	58,59,60,60	0
3	SO4	I	1803	5/5	0.87	0.36	67,67,70,70	0
4	GOL	N	2310	6/6	0.87	0.18	38,48,69,155	0
4	GOL	O	2410	6/6	0.87	0.21	47,53,59,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE	A	201	1/1	0.87	0.12	44,44,44,44	0
6	3PY	D	1310	6/7	0.87	0.19	50,63,70,78	0
3	SO4	A	1001	5/5	0.88	0.22	53,54,54,55	0
2	FE	D	201	1/1	0.88	0.09	46,46,46,46	0
4	GOL	J	1811	6/6	0.88	0.23	40,57,107,154	0
3	SO4	O	2406	5/5	0.88	0.20	41,44,46,47	5
4	GOL	F	1510	6/6	0.88	0.21	52,62,92,104	0
3	SO4	B	1101	5/5	0.88	0.17	66,66,67,67	0
3	SO4	B	1106	5/5	0.88	0.34	64,66,74,75	0
2	FE	F	201	1/1	0.88	0.06	46,46,46,46	0
3	SO4	H	1706	5/5	0.88	0.34	47,55,58,60	0
3	SO4	A	1105	5/5	0.89	0.47	51,53,55,61	0
3	SO4	N	2306	5/5	0.89	0.23	60,65,69,71	0
3	SO4	A	1006	5/5	0.89	0.36	56,67,69,74	0
3	SO4	C	1203	5/5	0.89	0.34	56,58,62,64	0
3	SO4	B	1104	5/5	0.90	0.15	73,73,74,75	0
3	SO4	H	1701	5/5	0.90	0.21	54,54,55,56	0
3	SO4	N	2303	5/5	0.90	0.50	64,68,70,72	0
4	GOL	B	1011	6/6	0.90	0.17	24,48,57,79	0
4	GOL	M	2210	6/6	0.90	0.25	34,50,95,99	0
3	SO4	A	1008	5/5	0.91	0.42	51,53,55,61	0
4	GOL	D	1211	6/6	0.91	0.12	45,49,55,68	0
3	SO4	I	1806	5/5	0.91	0.30	62,65,67,69	0
3	SO4	F	1506	5/5	0.91	0.25	65,67,68,69	0
3	SO4	L	2107	5/5	0.91	0.19	78,78,78,79	0
3	SO4	M	2201	5/5	0.91	0.18	51,51,52,53	0
2	FE	K	201	1/1	0.91	0.09	43,43,43,43	0
3	SO4	N	2301	5/5	0.91	0.21	62,63,63,63	0
3	SO4	F	1501	5/5	0.91	0.15	66,66,67,67	0
2	FE	G	201	1/1	0.92	0.08	43,43,43,43	0
4	GOL	K	2011	6/6	0.92	0.14	46,57,59,146	0
4	GOL	O	2411	6/6	0.92	0.10	26,52,74,76	0
2	FE	H	201	1/1	0.92	0.09	43,43,43,43	0
4	GOL	E	1410	6/6	0.92	0.24	39,50,75,155	0
2	FE	J	201	1/1	0.93	0.07	46,46,46,46	0
3	SO4	J	1904	5/5	0.93	0.21	61,61,62,63	5
2	FE	N	201	1/1	0.93	0.09	43,43,43,43	0
2	FE	C	201	1/1	0.93	0.08	46,46,46,46	0
3	SO4	B	1005	5/5	0.93	0.28	51,53,55,61	0
3	SO4	K	2003	5/5	0.93	0.29	69,69,69,71	0
2	FE	I	201	1/1	0.93	0.09	43,43,43,43	0
3	SO4	E	1406	5/5	0.94	0.22	62,67,67,70	0

Continued on next page...

Continued from previous page...

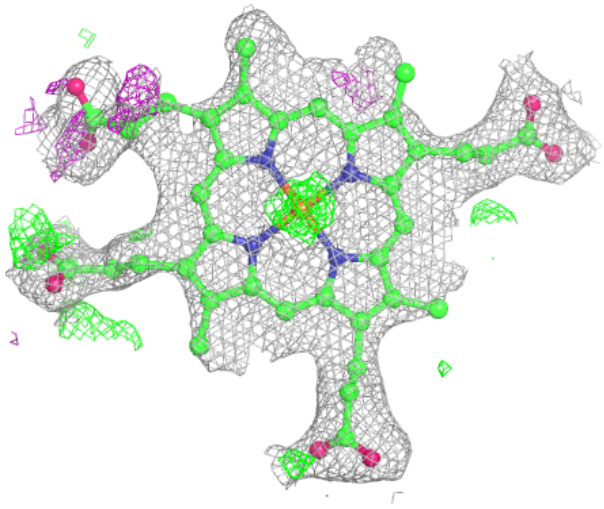
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	I	1801	5/5	0.94	0.17	61,61,62,63	0
2	FE	E	201	1/1	0.95	0.07	44,44,44,44	0
4	GOL	F	1512	6/6	0.95	0.14	22,37,47,49	0
3	SO4	K	2006	5/5	0.95	0.23	52,55,60,61	0
3	SO4	P	2506	5/5	0.95	0.24	57,63,66,67	0
3	SO4	I	1802	5/5	0.95	0.15	36,37,38,38	0
5	FEC	D	1311[A]	49/49	0.95	0.19	15,19,28,37	49
5	FEC	D	1311[B]	49/49	0.95	0.19	10,19,28,46	49
2	FE	P	201	1/1	0.95	0.05	45,45,45,45	0
5	FEC	B	1107[B]	49/49	0.96	0.20	15,18,27,38	49
2	FE	O	201	1/1	0.96	0.09	46,46,46,46	0
3	SO4	L	2102	5/5	0.96	0.16	78,78,78,79	5
5	FEC	F	1507[A]	49/49	0.96	0.17	15,19,29,36	49
5	FEC	F	1507[B]	49/49	0.96	0.17	16,19,31,38	49
5	FEC	G	1608[A]	49/49	0.96	0.19	15,18,28,37	49
5	FEC	G	1608[B]	49/49	0.96	0.19	10,17,29,38	49
5	FEC	P	2507[A]	49/49	0.96	0.17	15,18,28,37	49
5	FEC	P	2507[B]	49/49	0.96	0.17	16,18,28,33	49
5	FEC	B	1107[A]	49/49	0.96	0.20	15,18,28,37	49
5	FEC	L	2108[B]	49/49	0.97	0.19	13,18,28,39	49
5	FEC	M	2207[A]	49/49	0.97	0.18	14,18,28,37	49
5	FEC	M	2207[B]	49/49	0.97	0.18	13,18,27,39	49
5	FEC	I	1807[A]	49/49	0.97	0.18	15,19,28,37	49
5	FEC	I	1807[B]	49/49	0.97	0.18	14,19,27,38	49
5	FEC	L	2108[A]	49/49	0.97	0.19	15,18,28,37	49
2	FE	A	200	1/1	0.98	0.07	27,27,27,27	0
2	FE	K	200	1/1	0.99	0.06	28,28,28,28	0
2	FE	C	200	1/1	0.99	0.04	28,28,28,28	0
2	FE	L	200	1/1	0.99	0.07	26,26,26,26	0
2	FE	H	200	1/1	0.99	0.04	26,26,26,26	0
2	FE	M	200	1/1	0.99	0.07	26,26,26,26	0
2	FE	F	200	1/1	0.99	0.06	29,29,29,29	0
2	FE	N	200	1/1	0.99	0.05	25,25,25,25	0
2	FE	I	200	1/1	0.99	0.06	27,27,27,27	0
2	FE	O	200	1/1	0.99	0.07	29,29,29,29	0
2	FE	E	200	1/1	0.99	0.08	29,29,29,29	0
2	FE	P	200	1/1	0.99	0.05	28,28,28,28	0
2	FE	J	200	1/1	0.99	0.05	30,30,30,30	0
2	FE	G	200	1/1	0.99	0.06	26,26,26,26	0
2	FE	D	200	1/1	1.00	0.06	29,29,29,29	0
2	FE	B	200	1/1	1.00	0.07	25,25,25,25	0

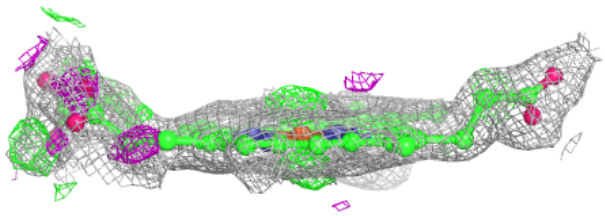
The following is a graphical depiction of the model fit to experimental electron density of all

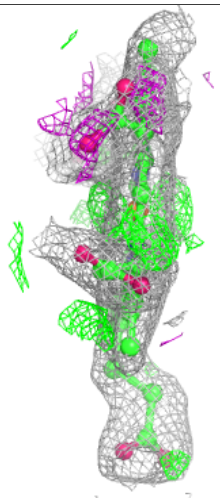
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FEC D 1311 (A):

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

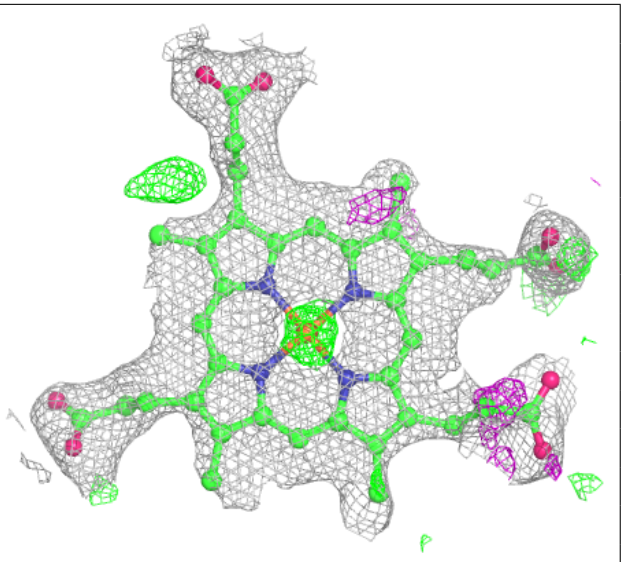


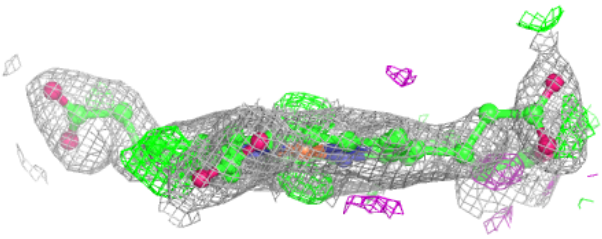


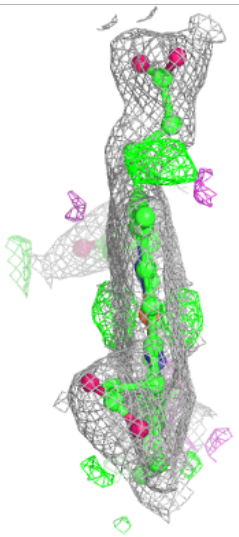


Electron density around FEC D 1311 (B):

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

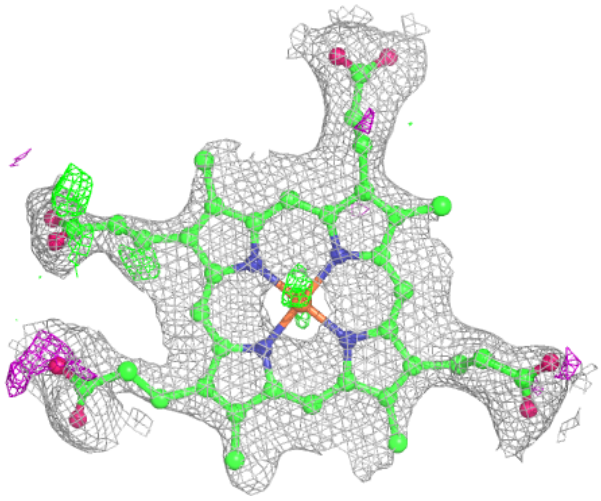


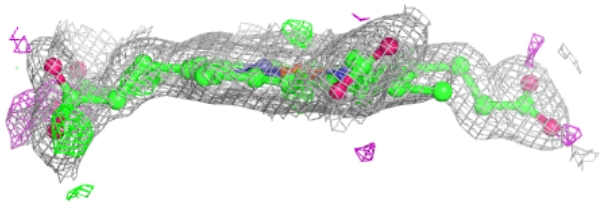


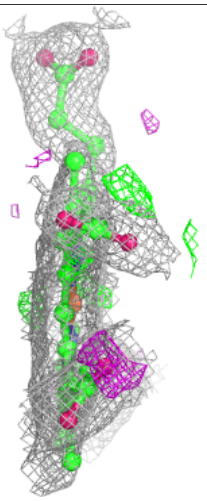


Electron density around FEC B 1107 (B):

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

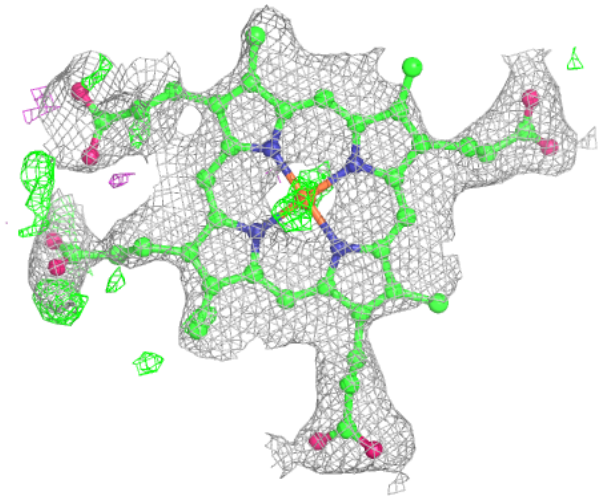


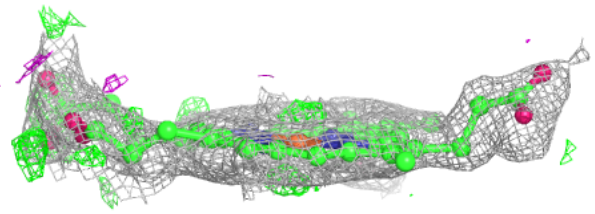


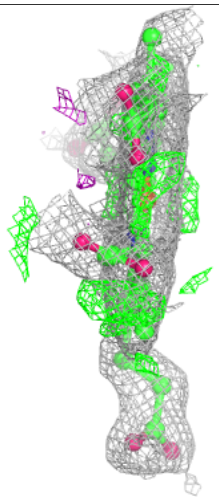


Electron density around FEC F 1507 (A):

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

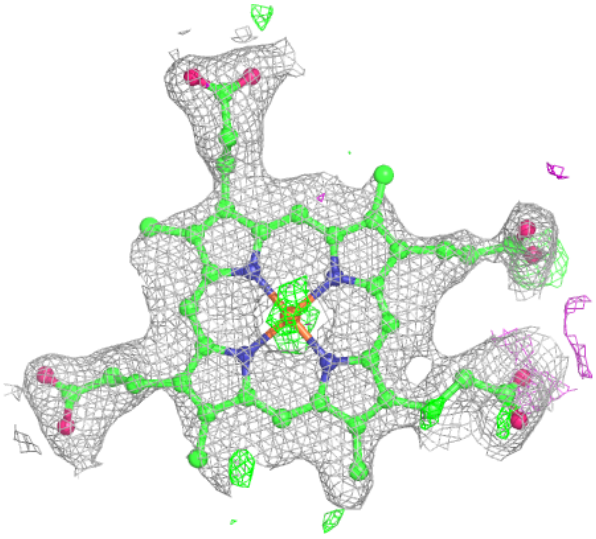


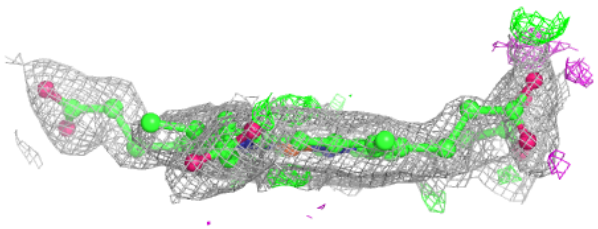


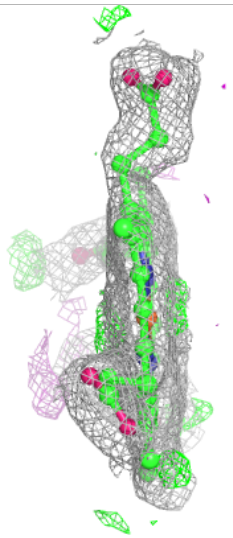


Electron density around FEC F 1507 (B):

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

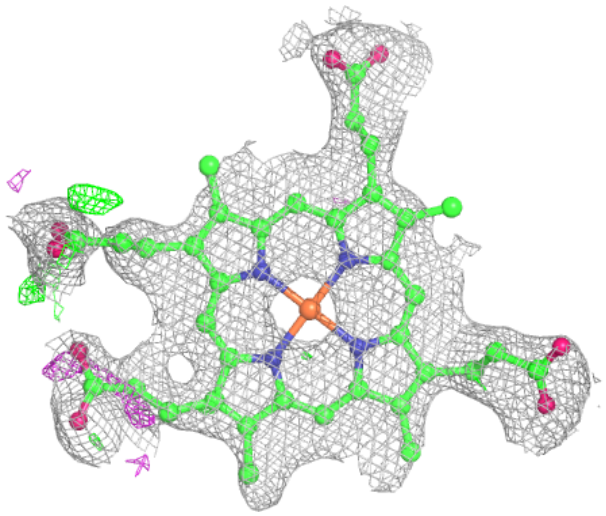


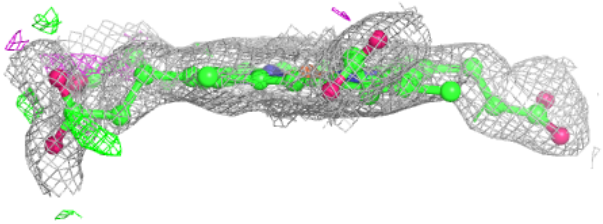


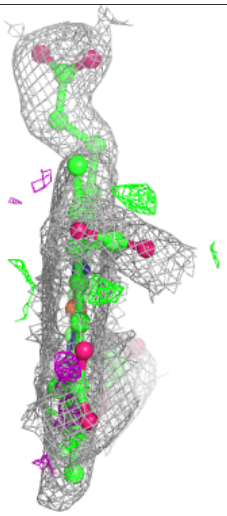


Electron density around FEC G 1608 (A):

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

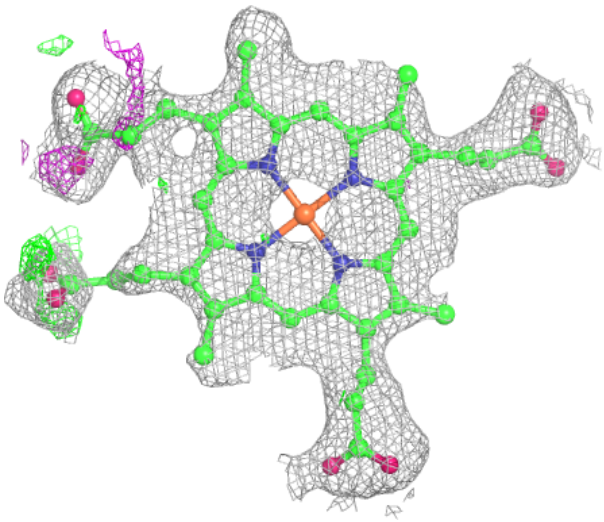


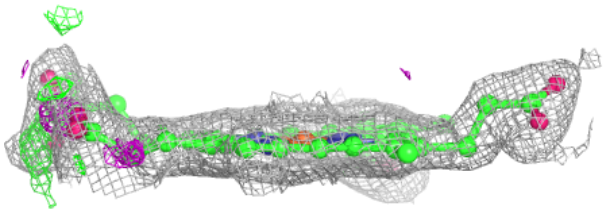


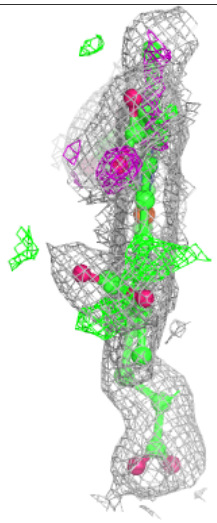


Electron density around FEC G 1608 (B):

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

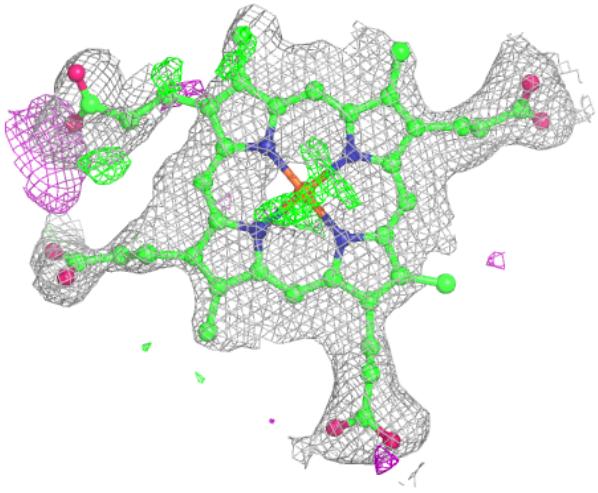


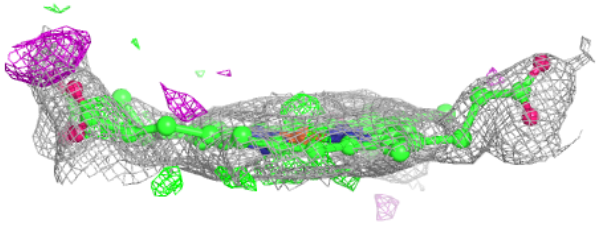


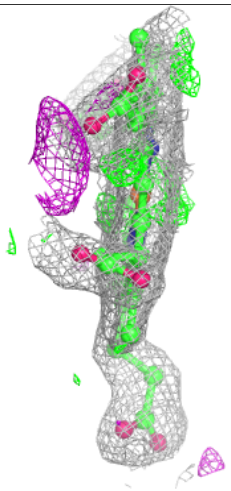


Electron density around FEC P 2507 (A):

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

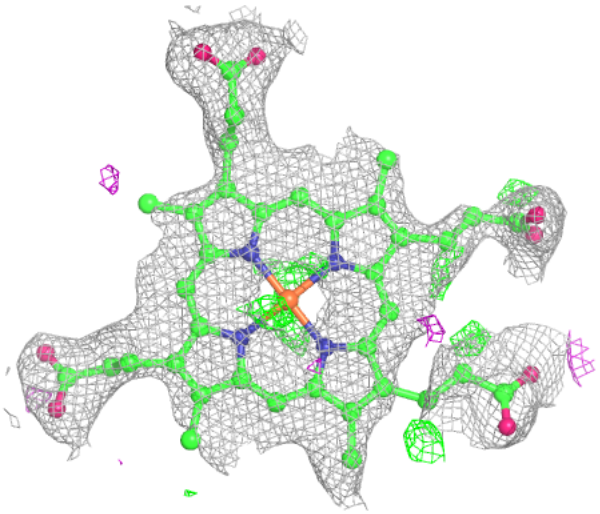


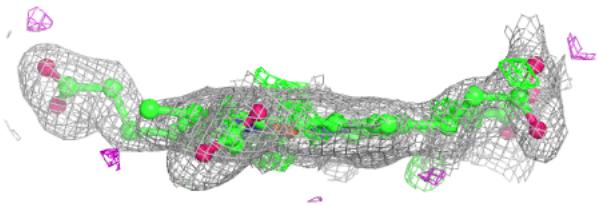


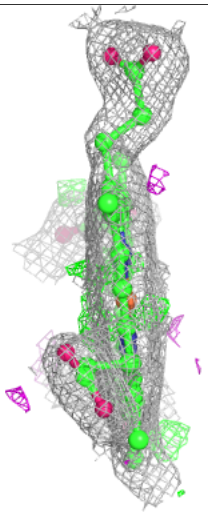


Electron density around FEC P 2507 (B):

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

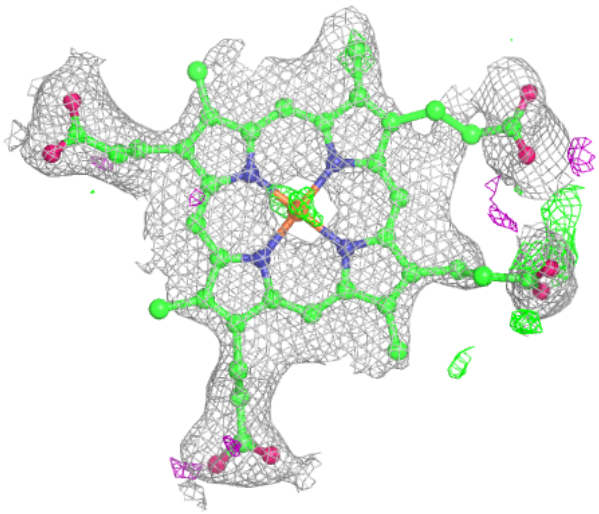


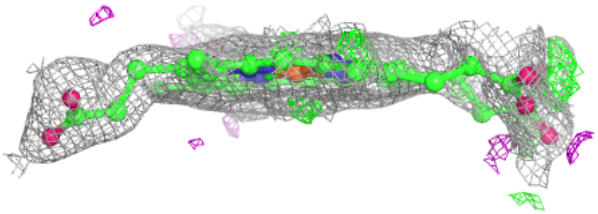


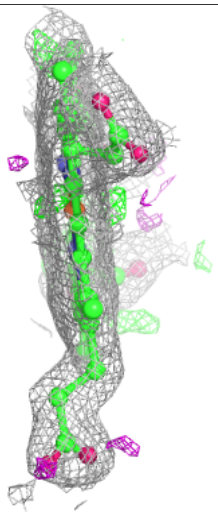


Electron density around FEC B 1107 (A):

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

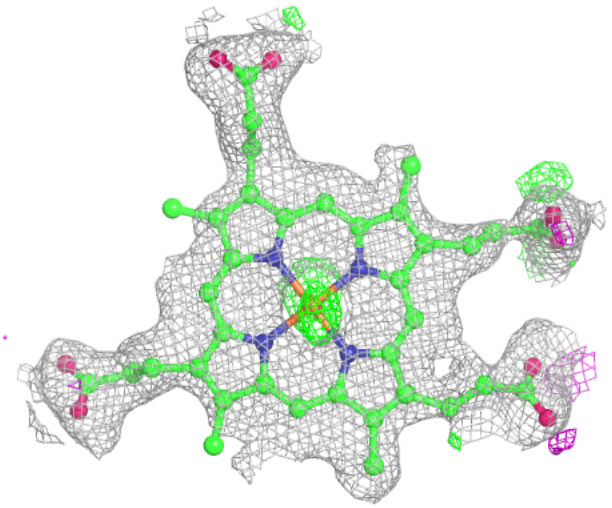


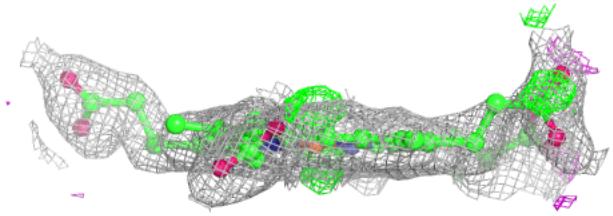


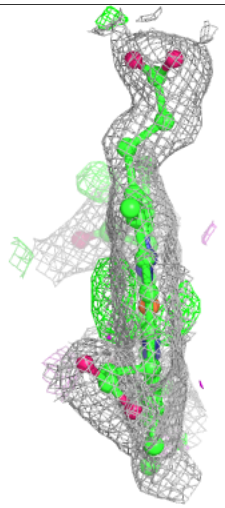


Electron density around FEC L 2108 (B):

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

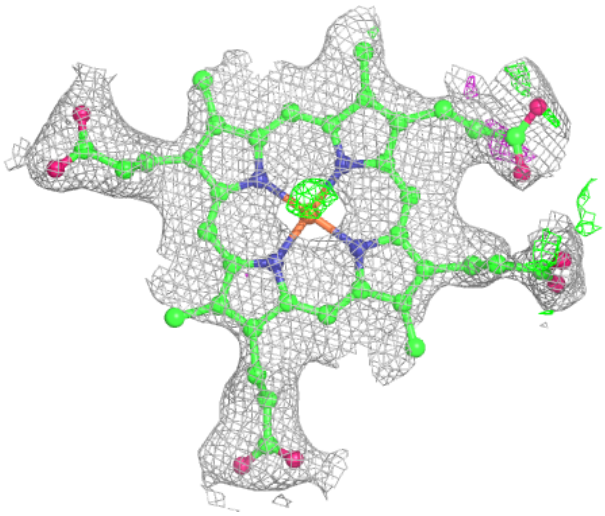


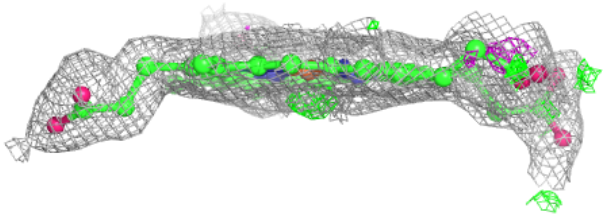


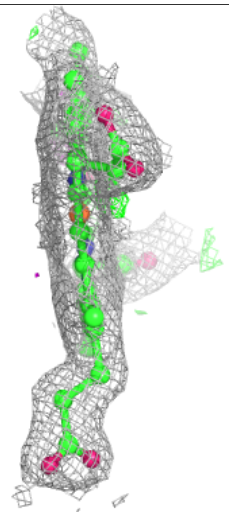


Electron density around FEC M 2207 (A):

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

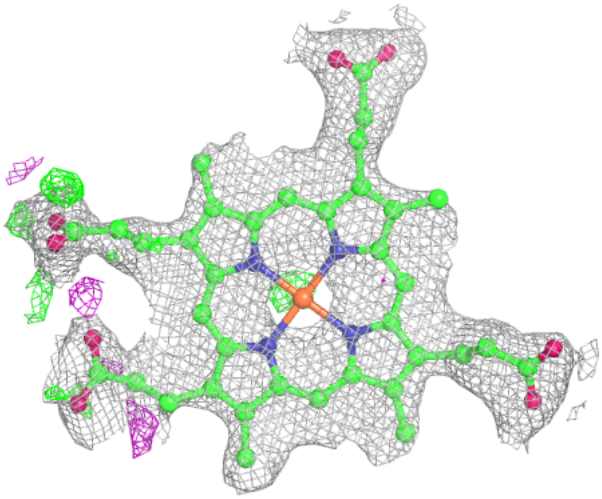


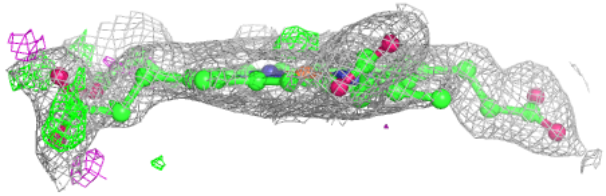


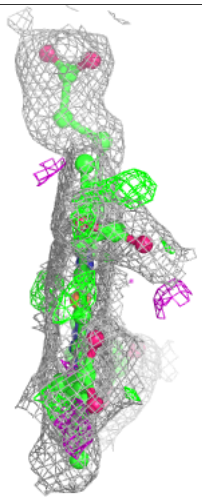


Electron density around FEC M 2207 (B):

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

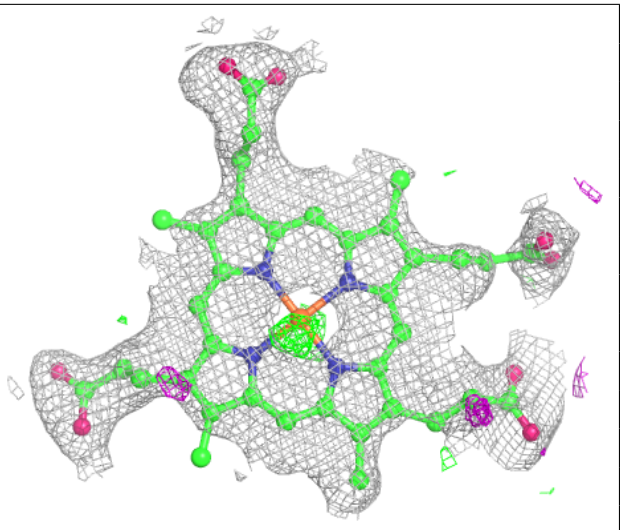


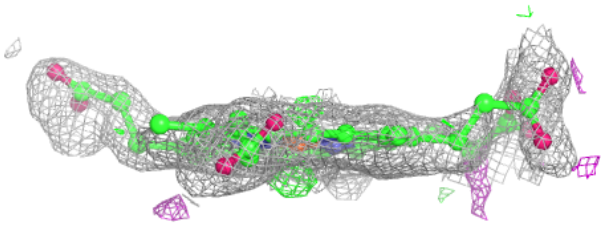


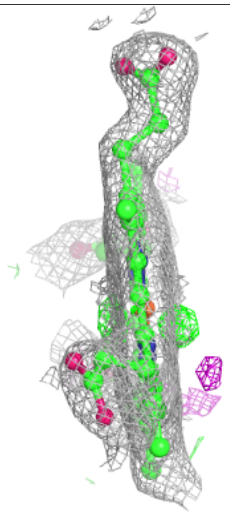


Electron density around FEC I 1807 (A):

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

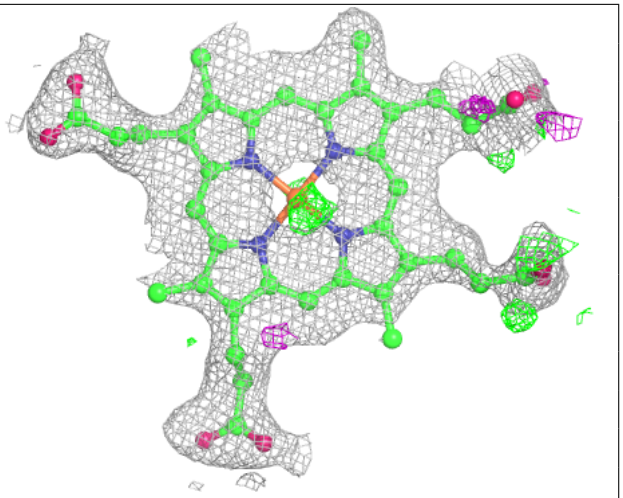


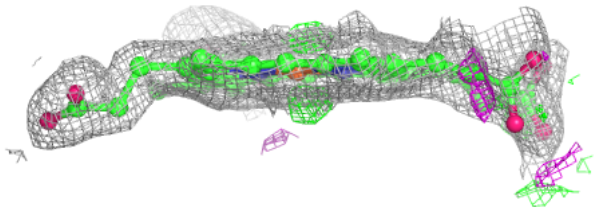


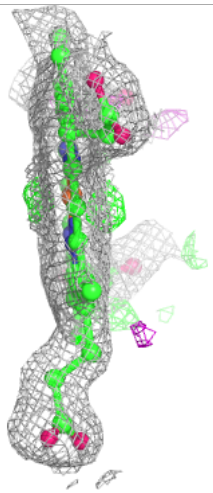


Electron density around FEC I 1807 (B):

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

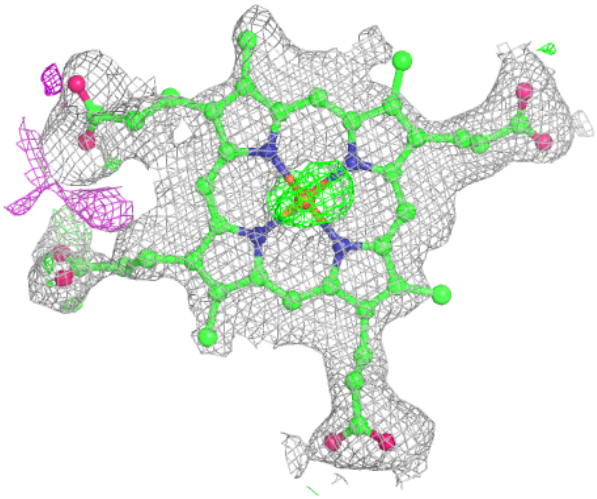


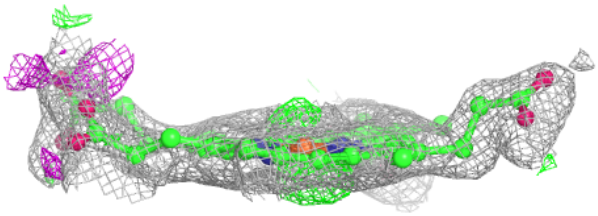


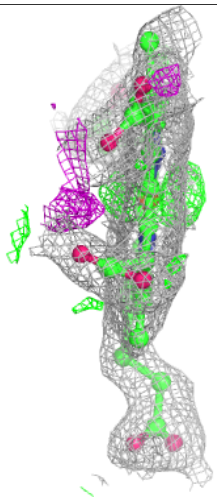


Electron density around FEC L 2108 (A):

$2mF_o$-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.