Full wwPDB X-ray Structure Validation Report (i)

Sep 11, 2023 – 06:59 PM EDT

PDB ID	:	4L3G
Title	:	Crystal Structure of the E113Q-MauG/pre-Methylamine Dehydrogenase Complex Aged 120 Days
Authors	:	Yukl, E.T.; Wilmot, C.M.
Deposited on	:	2013-06-05
Resolution	:	2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

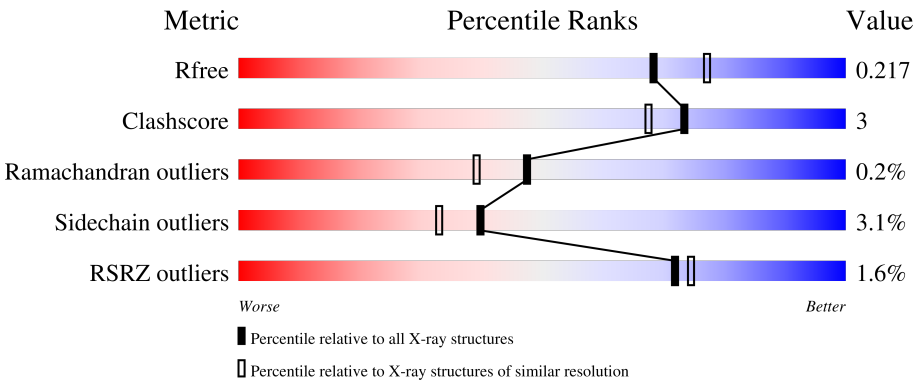
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	373	2%, 87%, 8%, • 5%
1	B	373	%, 87%, 8%, 5%
2	C	137	%, 79%, 11%, •• 9%
2	E	137	77%, 11%, • 9%
3	D	385	3%, 87%, 11%, •

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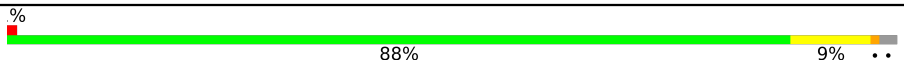
Mol	Chain	Length	Quality of chain
3	F	385	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 14591 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 Methylamine utilization protein MauG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	354	2741	1711	492	527	11	0	1	0
1	B	355	2787	1742	505	529	11	0	6	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	GLN	GLU	engineered mutation	UNP Q51658
A	368	HIS	-	expression tag	UNP Q51658
A	369	HIS	-	expression tag	UNP Q51658
A	370	HIS	-	expression tag	UNP Q51658
A	371	HIS	-	expression tag	UNP Q51658
A	372	HIS	-	expression tag	UNP Q51658
A	373	HIS	-	expression tag	UNP Q51658
B	113	GLN	GLU	engineered mutation	UNP Q51658
B	368	HIS	-	expression tag	UNP Q51658
B	369	HIS	-	expression tag	UNP Q51658
B	370	HIS	-	expression tag	UNP Q51658
B	371	HIS	-	expression tag	UNP Q51658
B	372	HIS	-	expression tag	UNP Q51658
B	373	HIS	-	expression tag	UNP Q51658

- Molecule 2 is a protein called methylamine dehydrogenase light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	125	958	592	161	191	14	0	1	0
2	E	125	962	596	161	191	14	0	2	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	132	HIS	-	expression tag	UNP A1BBA0
C	133	HIS	-	expression tag	UNP A1BBA0
C	134	HIS	-	expression tag	UNP A1BBA0
C	135	HIS	-	expression tag	UNP A1BBA0
C	136	HIS	-	expression tag	UNP A1BBA0
C	137	HIS	-	expression tag	UNP A1BBA0
E	132	HIS	-	expression tag	UNP A1BBA0
E	133	HIS	-	expression tag	UNP A1BBA0
E	134	HIS	-	expression tag	UNP A1BBA0
E	135	HIS	-	expression tag	UNP A1BBA0
E	136	HIS	-	expression tag	UNP A1BBA0
E	137	HIS	-	expression tag	UNP A1BBA0

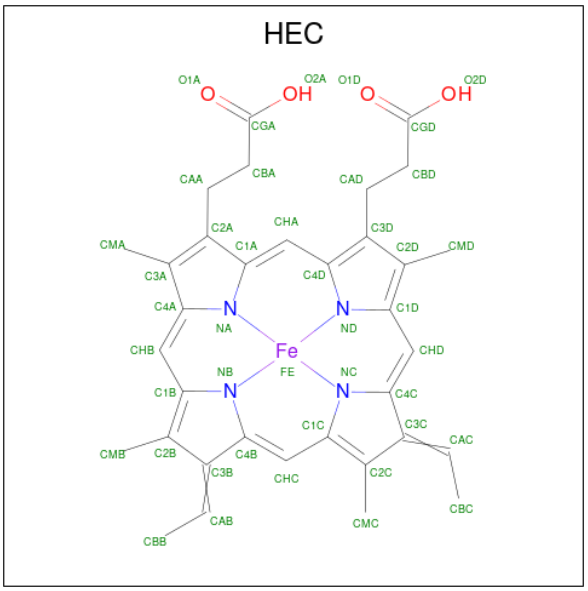
- Molecule 3 is a protein called methylamine dehydrogenase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	376	2933	1859	505	560	9	0	2	0
			Total	C	N	O	S			
3	F	376	2948	1872	507	561	8	0	4	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	1	1	1	0	0
			Total	Ca		
4	B	1	1	1	0	0

- Molecule 5 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).

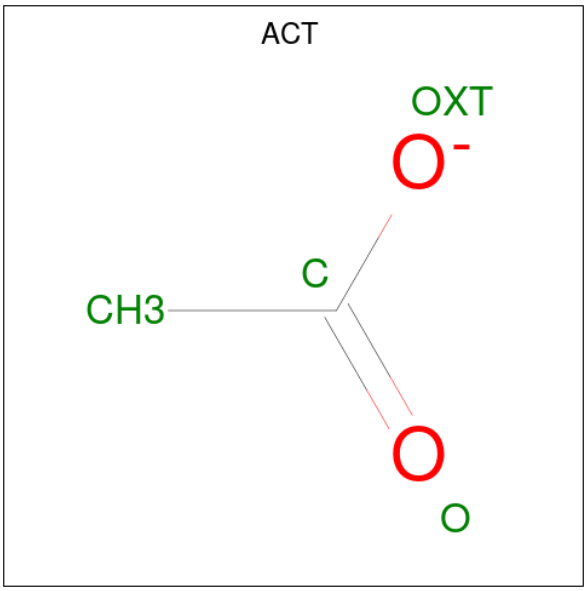


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
5	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	B	1	43	34	1	4	4	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

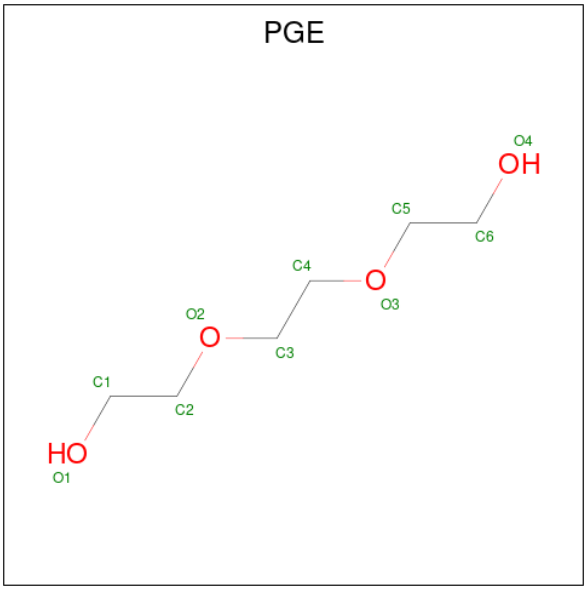
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
6	A	2	2	2	0	0
			Total	Na		
6	B	2	2	2	0	0

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	C	1	4	2	2	0	0
			Total	C	O		
7	F	1	4	2	2	0	0

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	F	1	10	6	4	0	0

- Molecule 9 is water.

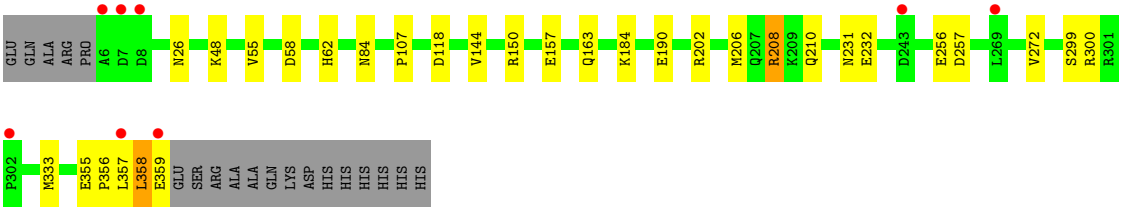
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	157	157	157	0	0
			Total	O		
9	B	239	239	239	0	0
			Total	O		
9	C	66	66	66	0	0
			Total	O		
9	D	203	204	204	0	1
			Total	O		
9	E	90	90	90	0	0
			Total	O		
9	F	308	310	310	0	2

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.

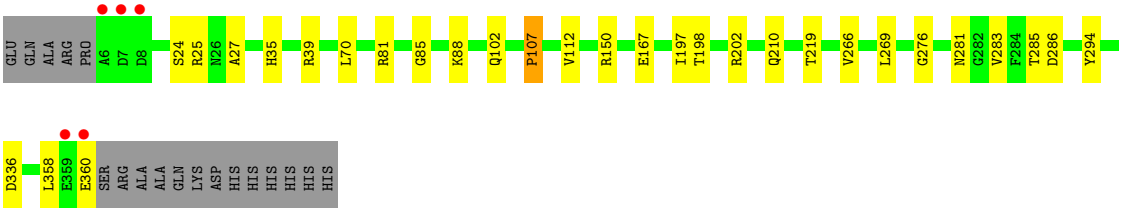
• Molecule 1: Methylamine utilization protein MauG

Chain A:



• Molecule 1: Methylamine utilization protein MauG

Chain B:



• Molecule 2: methylamine dehydrogenase light chain

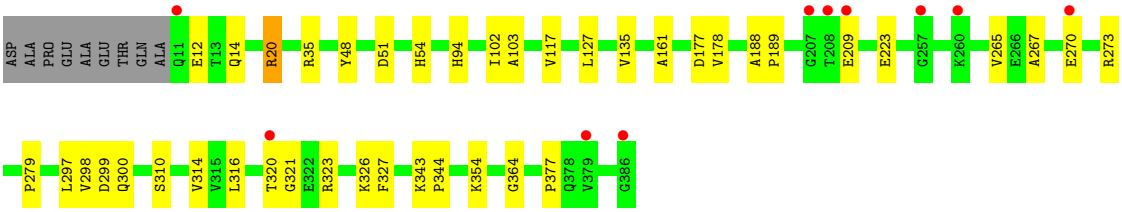
Chain C:

• Molecule 2: methylamine dehydrogenase light chain

Chain E:

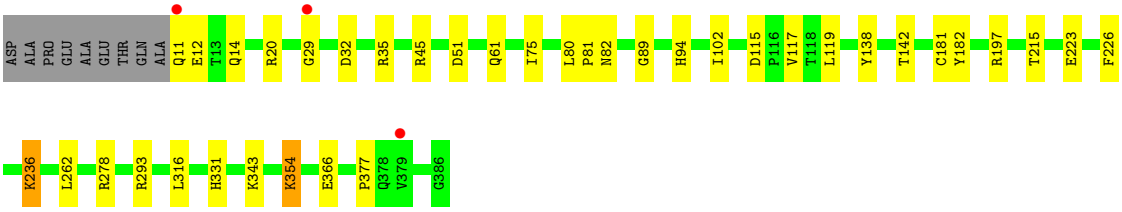
• Molecule 3: methylamine dehydrogenase heavy chain

Chain D:



- Molecule 3: methylamine dehydrogenase heavy chain

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	55.53Å 83.52Å 107.78Å 109.94° 91.54° 105.78°	Depositor
Resolution (Å)	29.62 – 2.05 29.62 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.62-2.05) 97.8 (29.62-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.158 , 0.210 0.165 , 0.217	Depositor DCC
R_{free} test set	5334 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	31.1	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14591	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HYP, PGE, ACT, CA, TRQ, NA, HEC

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	0.85	0/2798	0.87	4/3794 (0.1%)
1	B	0.91	1/2859 (0.0%)	0.91	2/3873 (0.1%)
2	C	0.91	0/969	0.92	2/1323 (0.2%)
2	E	1.04	0/976	0.97	1/1333 (0.1%)
3	D	0.85	1/3017 (0.0%)	0.88	1/4110 (0.0%)
3	F	1.01	0/3037	1.01	7/4136 (0.2%)
All	All	0.92	2/13656 (0.0%)	0.92	17/18569 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	C	0	4
2	E	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	294	TYR	CE1-CZ	-5.44	1.31	1.38
3	D	48	TYR	CG-CD1	5.21	1.46	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	257	ASP	CB-CG-OD2	-7.98	111.12	118.30
1	A	257	ASP	CB-CG-OD1	6.91	124.52	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	236[A]	LYS	CA-C-O	6.28	133.29	120.10
3	F	236[B]	LYS	CA-C-O	6.28	133.29	120.10
3	F	138	TYR	CB-CG-CD1	5.98	124.59	121.00
2	C	19	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	58	ASP	CB-CG-OD2	-5.63	113.24	118.30
1	B	150	ARG	NE-CZ-NH1	5.60	123.10	120.30
3	F	197	ARG	NE-CZ-NH2	5.55	123.07	120.30
2	E	99	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	336	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	58	ASP	CB-CG-OD1	5.32	123.09	118.30
3	F	236[A]	LYS	N-CA-C	5.07	124.68	111.00
3	F	236[B]	LYS	N-CA-C	5.07	124.68	111.00
2	C	8	ASP	CB-CG-OD1	5.04	122.84	118.30
3	D	35	ARG	NE-CZ-NH1	5.01	122.81	120.30
3	F	35	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	107	HYP	Mainchain
2	C	108	TRP	Mainchain
2	C	56	SER	Mainchain,Peptide
2	C	57	TRQ	Mainchain
2	E	56	SER	Mainchain

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	2741	0	2617	13	0
1	B	2787	0	2692	16	0
2	C	958	0	862	9	0
2	E	962	0	871	15	0
3	D	2933	0	2821	18	0
3	F	2948	0	2852	20	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	86	0	60	3	0
5	B	86	0	60	3	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	C	4	0	3	1	0
7	F	4	0	3	0	0
8	F	10	0	14	0	0
9	A	157	0	0	1	0
9	B	239	0	0	2	0
9	C	66	0	0	1	0
9	D	204	0	0	2	0
9	E	90	0	0	3	0
9	F	310	0	0	6	0
All	All	14591	0	12855	85	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (85) 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:B:210:GLN:HE22	2:E:44:THR:HG21	1.52	0.74
1:A:208:ARG:NH2	3:F:29:GLY:O	2.23	0.71
2:C:21:GLN:HE22	3:F:14:GLN:HE21	1.39	0.69
1:A:210:GLN:HE22	2:C:44:THR:HG21	1.59	0.66
3:D:297:LEU:HD22	3:D:310:SER:HB2	1.77	0.65
1:B:285:THR:HG22	1:B:286:ASP:OD1	1.97	0.65
1:B:198:THR:HG22	2:E:58[A]:VAL:HG13	1.78	0.64
7:C:201:ACT:H3	9:C:318:HOH:O	1.97	0.64
3:D:314:VAL:HG12	3:D:326:LYS:HG3	1.80	0.62
5:B:402:HEC:HBB3	5:B:402:HEC:HMB1	1.83	0.60
5:A:402:HEC:HBC3	5:A:402:HEC:HMC1	1.83	0.60
3:F:12:GLU:OE2	3:F:20:ARG:NH1	2.34	0.60
3:F:278:ARG:NH1	9:F:621:HOH:O	2.25	0.60
3:F:236[A]:LYS:NZ	9:F:785:HOH:O	2.36	0.59
1:B:39[A]:ARG:NH2	1:B:276:GLY:O	2.34	0.59
1:A:231:ASN:OD1	1:A:231:ASN:C	2.40	0.57
3:F:12:GLU:OE1	3:F:20:ARG:NH1	2.38	0.56
1:B:197:ILE:O	1:B:202:ARG:CD	2.54	0.55
3:D:12:GLU:OE1	3:D:20[A]:ARG:NH1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:57:TRQ:HB2	2:C:108:TRP:NE1	2.22	0.54
3:D:265:VAL:HG21	3:D:321:GLY:HA2	1.90	0.54
1:A:357:LEU:O	1:A:359:GLU:N	2.41	0.54
3:D:54:HIS:HD2	9:D:585:HOH:O	1.91	0.53
1:A:144:VAL:HA	1:A:150:ARG:NH1	2.23	0.53
3:F:181:CYS:C	3:F:182:TYR:CD1	2.82	0.53
2:E:95:LEU:HD22	3:F:226:PHE:CE1	2.44	0.52
1:B:281:ASN:OD1	1:B:283:VAL:HB	2.08	0.52
3:D:14:GLN:HE21	2:E:21:GLN:HE22	1.57	0.52
3:F:115:ASP:O	3:F:119:LEU:HA	2.10	0.52
3:D:20[A]:ARG:HG2	9:D:545:HOH:O	2.09	0.52
3:D:188:ALA:HB1	3:D:189:PRO:HD2	1.92	0.52
1:B:81[B]:ARG:CZ	1:B:85:GLY:HA2	2.41	0.51
1:A:163:GLN:HE22	5:A:402:HEC:HMA1	1.75	0.51
3:F:51:ASP:HA	3:F:377:PRO:HA	1.93	0.51
3:F:45:ARG:NH2	3:F:343:LYS:O	2.44	0.50
1:A:26:ASN:ND2	9:A:583:HOH:O	2.44	0.50
1:B:197:ILE:O	1:B:202:ARG:HD2	2.12	0.50
3:D:270:GLU:HA	3:D:273:ARG:NH1	2.26	0.50
1:A:55:VAL:HG22	1:A:62:HIS:CE1	2.47	0.50
1:B:210:GLN:NE2	2:E:44:THR:HG21	2.25	0.49
2:E:56:SER:CB	2:E:74:TYR:O	2.61	0.49
2:C:23:CYS:HB3	2:C:88[B]:CYS:SG	2.53	0.48
2:E:75:ARG:HD2	9:E:276:HOH:O	2.13	0.48
2:E:131:SER:HB2	9:E:268:HOH:O	2.13	0.47
2:E:56:SER:HB3	2:E:74:TYR:O	2.15	0.47
1:A:272:VAL:HG21	5:A:403:HEC:HMA3	1.96	0.47
3:D:103:ALA:HB3	9:F:704:HOH:O	2.15	0.45
1:A:357:LEU:C	1:A:359:GLU:H	2.19	0.45
2:E:57:TRQ:HB2	2:E:108:TRP:NE1	2.31	0.44
3:F:80:LEU:N	3:F:81:PRO:HD3	2.32	0.44
3:D:327:PHE:CD1	3:D:364:GLY:HA3	2.53	0.44
2:E:101:GLU:HA	9:E:272:HOH:O	2.18	0.44
2:C:86:CYS:N	2:C:87:PRO:CD	2.81	0.44
3:D:343:LYS:N	3:D:344:PRO:CD	2.81	0.43
2:C:20:ILE:HG22	2:C:25:TYR:CZ	2.53	0.43
3:F:354:LYS:NZ	9:F:676:HOH:O	2.51	0.43
2:E:58[B]:VAL:HG22	2:E:59:ALA:N	2.33	0.43
3:F:182:TYR:CD1	3:F:182:TYR:N	2.87	0.43
1:A:299:SER:HB2	1:A:333:MET:HG3	2.00	0.43
1:B:197:ILE:O	1:B:202:ARG:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:THR:CG2	2:E:58[A]:VAL:HG13	2.48	0.43
3:F:12:GLU:CD	3:F:20:ARG:NH1	2.72	0.43
1:A:355:GLU:N	1:A:356:PRO:CD	2.82	0.42
1:A:48:LYS:H	1:A:62:HIS:CE1	2.38	0.42
3:D:279:PRO:HA	3:D:298:VAL:HA	2.01	0.42
1:B:360:GLU:C	9:B:726:HOH:O	2.58	0.42
3:D:299:ASP:OD1	3:D:300:GLN:N	2.50	0.42
3:F:331:HIS:HE1	3:F:366:GLU:OE1	2.03	0.42
3:F:215:THR:HG21	9:F:679:HOH:O	2.19	0.42
1:B:24:SER:OG	1:B:27:ALA:HA	2.19	0.41
2:E:71:LEU:HD22	2:E:129:LYS:O	2.19	0.41
3:F:82:ASN:HB3	3:F:142:THR:HB	2.01	0.41
2:E:77:CYS:O	2:E:120:HIS:HB3	2.20	0.41
3:D:51:ASP:HA	3:D:377:PRO:HA	2.03	0.41
2:C:23:CYS:CB	2:C:88[B]:CYS:SG	3.09	0.41
2:C:106:ILE:HA	3:D:135:VAL:HG23	2.01	0.41
1:B:35:HIS:CE1	1:B:70:LEU:HD21	2.56	0.41
3:F:89:GLY:HA2	9:F:505:HOH:O	2.21	0.41
1:B:25:ARG:NH1	9:B:718:HOH:O	2.48	0.40
1:B:266:VAL:HG22	5:B:403:HEC:HMD3	2.02	0.40
3:D:161:ALA:HA	3:D:178:VAL:HG22	2.03	0.40
3:D:267:ALA:O	3:D:323:ARG:NH2	2.51	0.40
2:C:80:TYR:HB2	2:C:120:HIS:HB2	2.04	0.40
3:F:61:GLN:HB3	3:F:75[A]:ILE:HB	2.03	0.40
5:B:402:HEC:HBB3	5:B:402:HEC:CMB	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	352/373 (94%)	339 (96%)	12 (3%)	1 (0%)	41 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	358/373 (96%)	346 (97%)	12 (3%)	0	100	100
2	C	123/137 (90%)	120 (98%)	3 (2%)	0	100	100
2	E	124/137 (90%)	120 (97%)	4 (3%)	0	100	100
3	D	376/385 (98%)	362 (96%)	13 (4%)	1 (0%)	41	31
3	F	377/385 (98%)	363 (96%)	12 (3%)	2 (0%)	29	18
All	All	1710/1790 (96%)	1650 (96%)	56 (3%)	4 (0%)	47	39

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	358	LEU
3	D	102	ILE
3	F	32	ASP
3	F	102	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	276/291 (95%)	264 (96%)	12 (4%)	29	22
1	B	282/291 (97%)	274 (97%)	8 (3%)	43	37
2	C	105/112 (94%)	104 (99%)	1 (1%)	76	75
2	E	106/112 (95%)	102 (96%)	4 (4%)	33	26
3	D	306/310 (99%)	295 (96%)	11 (4%)	35	28
3	F	308/310 (99%)	299 (97%)	9 (3%)	42	35
All	All	1383/1426 (97%)	1338 (97%)	45 (3%)	40	31

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	118	ASP

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Mol	Chain	Res	Type
1	A	157	GLU
1	A	184	LYS
1	A	190	GLU
1	A	202	ARG
1	A	206	MET
1	A	208	ARG
1	A	232	GLU
1	A	256	GLU
1	A	300	ARG
1	A	358	LEU
1	B	88	LYS
1	B	102	GLN
1	B	112	VAL
1	B	167	GLU
1	B	219	THR
1	B	269[A]	LEU
1	B	269[B]	LEU
1	B	358	LEU
2	C	71	LEU
3	D	20[A]	ARG
3	D	20[B]	ARG
3	D	94	HIS
3	D	117	VAL
3	D	127	LEU
3	D	177	ASP
3	D	209	GLU
3	D	223	GLU
3	D	316	LEU
3	D	320	THR
3	D	354	LYS
2	E	7	THR
2	E	16	GLN
2	E	71	LEU
2	E	131	SER
3	F	11[A]	GLN
3	F	11[B]	GLN
3	F	94	HIS
3	F	117	VAL
3	F	223	GLU
3	F	262	LEU
3	F	293	ARG
3	F	316	LEU

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Mol	Chain	Res	Type
3	F	354	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	29	GLN
1	A	62	HIS
1	A	91	GLN
1	A	163	GLN
1	A	210	GLN
1	B	16	GLN
1	B	91	GLN
1	B	163	GLN
1	B	210	GLN
2	E	21	GLN
2	E	68	GLN
3	F	14	GLN
3	F	54	HIS
3	F	300	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	HYP	A	107	1	6,8,9	1.10	0	5,10,12	2.17	2 (40%)
2	TRQ	E	57	2	13,17,18	2.71	7 (53%)	14,24,26	3.19	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	HYP	B	107	1	6,8,9	0.95	0	5,10,12	2.29	3 (60%)
2	TRQ	C	57	2	13,17,18	2.70	4 (30%)	14,24,26	3.44	5 (35%)

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
1	HYP	A	107	1	-	0/0/11/13	0/1/1/1
2	TRQ	E	57	2	-	0/4/19/21	0/2/2/2
1	HYP	B	107	1	-	0/0/11/13	0/1/1/1
2	TRQ	C	57	2	-	0/4/19/21	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	57	TRQ	CH2-CZ2	-7.04	1.46	1.54
2	E	57	TRQ	CH2-CZ2	-5.57	1.47	1.54
2	E	57	TRQ	CD2-CE3	4.99	1.55	1.44
2	C	57	TRQ	CD2-CE3	3.92	1.53	1.44
2	E	57	TRQ	CD1-NE1	-3.63	1.30	1.36
2	C	57	TRQ	CZ3-CE3	3.44	1.40	1.34
2	E	57	TRQ	CZ3-CE3	3.29	1.40	1.34
2	E	57	TRQ	CZ3-CH2	-2.53	1.39	1.45
2	C	57	TRQ	CD1-NE1	-2.04	1.33	1.36
2	E	57	TRQ	CE2-CZ2	-2.02	1.47	1.50
2	E	57	TRQ	O-C	2.00	1.27	1.19

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	57	TRQ	CB-CG-CD1	-9.76	115.91	127.97
2	E	57	TRQ	CB-CG-CD1	-9.10	116.73	127.97
2	E	57	TRQ	CZ2-CE2-NE1	5.35	128.48	119.94
2	C	57	TRQ	CZ2-CE2-NE1	4.80	127.60	119.94
2	C	57	TRQ	O6-CH2-CZ2	-3.75	115.95	118.51
1	A	107	HYP	CG-CB-CA	3.66	108.59	103.96
2	C	57	TRQ	CB-CG-CD2	3.52	134.75	127.09
2	E	57	TRQ	O7-CZ2-CE2	-3.34	118.31	121.84
1	B	107	HYP	O-C-CA	-3.19	116.41	124.78
2	E	57	TRQ	CB-CG-CD2	3.14	133.93	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	107	HYP	CG-CB-CA	2.75	107.43	103.96
2	C	57	TRQ	CB-CA-C	2.74	116.61	111.47
1	B	107	HYP	CB-CG-CD	2.51	106.35	103.27
1	A	107	HYP	OD1-CG-CD	2.22	115.19	110.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	57	TRQ	1	0
2	C	57	TRQ	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
5	HEC	A	402	1	32,50,50	1.94	8 (25%)	24,82,82	2.20	10 (41%)
7	ACT	F	401	-	3,3,3	0.87	0	3,3,3	1.03	0
7	ACT	C	201	-	3,3,3	1.07	0	3,3,3	0.38	0
5	HEC	B	402	1	32,50,50	1.58	9 (28%)	24,82,82	2.50	13 (54%)
8	PGE	F	402	-	9,9,9	0.62	0	8,8,8	0.54	0
5	HEC	A	403	1	32,50,50	1.67	7 (21%)	24,82,82	2.36	7 (29%)
5	HEC	B	403	1	32,50,50	1.55	5 (15%)	24,82,82	1.97	10 (41%)

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
5	HEC	A	402	1	-	0/10/54/54	-
5	HEC	B	402	1	-	0/10/54/54	-
8	PGE	F	402	-	-	3/7/7/7	-
5	HEC	A	403	1	-	2/10/54/54	-
5	HEC	B	403	1	-	2/10/54/54	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	402	HEC	C3C-C2C	-4.48	1.36	1.40
5	A	403	HEC	C2B-C3B	-4.07	1.36	1.40
5	B	403	HEC	C3C-C2C	-3.84	1.36	1.40
5	A	402	HEC	C2A-C1A	3.62	1.50	1.42
5	A	402	HEC	C2B-C3B	-3.59	1.37	1.40
5	A	402	HEC	C3C-C4C	3.41	1.49	1.43
5	B	402	HEC	C2A-C1A	3.25	1.49	1.42
5	A	402	HEC	C3A-C4A	3.23	1.49	1.42
5	A	403	HEC	C3C-C4C	3.22	1.48	1.43
5	A	403	HEC	C1B-NB	-2.85	1.30	1.36
5	B	403	HEC	C3C-C4C	2.81	1.48	1.43
5	A	402	HEC	C4B-C3B	2.77	1.48	1.43
5	A	403	HEC	C1C-NC	-2.74	1.30	1.36
5	B	402	HEC	C3C-C2C	-2.74	1.37	1.40
5	B	402	HEC	C3A-C4A	2.69	1.48	1.42
5	A	403	HEC	C4D-CHA	2.67	1.48	1.41
5	B	403	HEC	C3A-C4A	2.59	1.48	1.42
5	B	402	HEC	C2B-C3B	-2.45	1.38	1.40
5	B	402	HEC	C1B-CHB	2.43	1.47	1.41
5	B	402	HEC	C1D-CHD	2.37	1.47	1.41
5	A	402	HEC	C1D-CHD	2.32	1.47	1.41
5	B	402	HEC	C1C-NC	-2.27	1.31	1.36
5	A	403	HEC	C3A-C4A	2.18	1.47	1.42
5	B	403	HEC	C1B-NB	-2.15	1.31	1.36
5	A	402	HEC	C4D-CHA	2.12	1.46	1.41
5	B	402	HEC	C1C-CHC	2.11	1.46	1.41
5	B	402	HEC	C4B-C3B	2.11	1.46	1.43
5	A	403	HEC	C2A-C1A	2.05	1.47	1.42
5	B	403	HEC	C2B-C3B	-2.02	1.38	1.40

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	403	HEC	CBD-CAD-C3D	-6.67	101.23	112.62
5	A	402	HEC	C1D-C2D-C3D	-5.80	102.96	107.00
5	A	403	HEC	CMC-C2C-C3C	4.44	131.04	125.82
5	A	402	HEC	CBD-CAD-C3D	-4.42	105.08	112.62
5	B	402	HEC	CBD-CAD-C3D	-4.38	105.15	112.62
5	B	402	HEC	CMB-C2B-C3B	4.10	130.64	125.82
5	A	403	HEC	C4C-C3C-C2C	-4.06	101.97	106.35
5	B	402	HEC	CMC-C2C-C3C	3.96	130.48	125.82
5	B	403	HEC	CBD-CAD-C3D	-3.96	105.87	112.62
5	B	402	HEC	C2B-C3B-C4B	-3.73	102.32	106.35
5	B	403	HEC	C4C-C3C-C2C	-3.72	102.33	106.35
5	A	403	HEC	C1D-C2D-C3D	-3.37	104.65	107.00
5	B	403	HEC	CBA-CAA-C2A	-3.29	107.06	112.60
5	A	403	HEC	CBA-CAA-C2A	-3.28	107.07	112.60
5	B	402	HEC	C1D-C2D-C3D	-3.25	104.73	107.00
5	B	402	HEC	C4C-C3C-C2C	-3.24	102.85	106.35
5	A	402	HEC	C4C-C3C-C2C	-3.05	103.06	106.35
5	B	403	HEC	C1D-C2D-C3D	-2.93	104.95	107.00
5	B	403	HEC	CMB-C2B-C3B	2.92	129.26	125.82
5	B	402	HEC	CMB-C2B-C1B	-2.86	124.06	128.46
5	A	403	HEC	C2B-C3B-C4B	-2.83	103.30	106.35
5	A	402	HEC	C2B-C3B-C4B	-2.65	103.49	106.35
5	A	403	HEC	CMC-C2C-C1C	-2.64	124.41	128.46
5	B	403	HEC	C3C-C4C-NC	2.63	115.90	110.94
5	B	402	HEC	C3B-C4B-NB	2.58	115.81	110.94
5	B	402	HEC	O2D-CGD-CBD	2.56	122.25	114.03
5	B	402	HEC	O2A-CGA-CBA	2.41	121.78	114.03
5	B	402	HEC	CMD-C2D-C3D	2.37	129.41	124.94
5	B	402	HEC	CMA-C3A-C2A	2.33	129.34	124.94
5	A	402	HEC	C3C-C4C-NC	2.26	115.20	110.94
5	B	403	HEC	CMC-C2C-C3C	2.22	128.43	125.82
5	A	402	HEC	O2A-CGA-CBA	2.21	121.13	114.03
5	B	402	HEC	CMC-C2C-C1C	-2.20	125.08	128.46
5	A	402	HEC	CBA-CAA-C2A	-2.17	108.94	112.60
5	B	403	HEC	CMB-C2B-C1B	-2.16	125.15	128.46
5	A	402	HEC	CMA-C3A-C2A	2.15	129.00	124.94
5	B	403	HEC	C2B-C3B-C4B	-2.13	104.05	106.35
5	B	403	HEC	CMA-C3A-C2A	2.07	128.84	124.94
5	A	402	HEC	CMB-C2B-C3B	2.07	128.25	125.82
5	A	402	HEC	CMC-C2C-C3C	2.01	128.19	125.82

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	402	PGE	O3-C5-C6-O4
8	F	402	PGE	O1-C1-C2-O2
8	F	402	PGE	O2-C3-C4-O3
5	B	403	HEC	CAD-CBD-CGD-O2D
5	B	403	HEC	CAD-CBD-CGD-O1D
5	A	403	HEC	CAD-CBD-CGD-O2D
5	A	403	HEC	CAD-CBD-CGD-O1D

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	402	HEC	2	0
7	C	201	ACT	1	0
5	B	402	HEC	2	0
5	A	403	HEC	1	0
5	B	403	HEC	1	0

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

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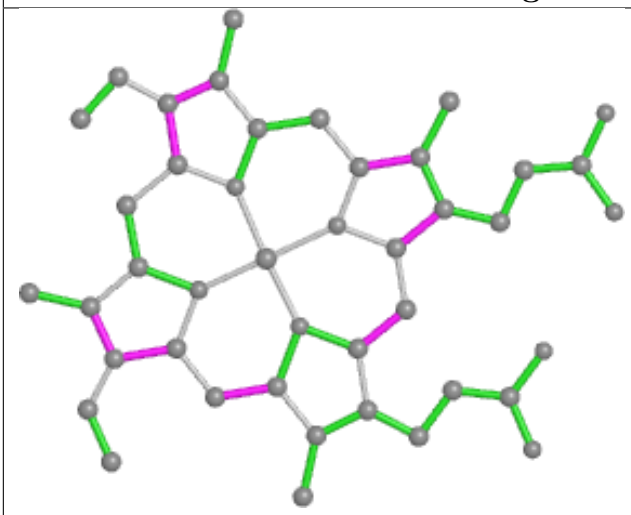
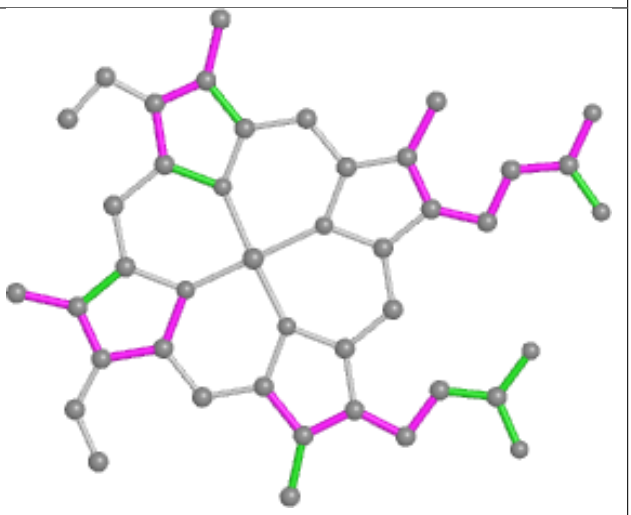
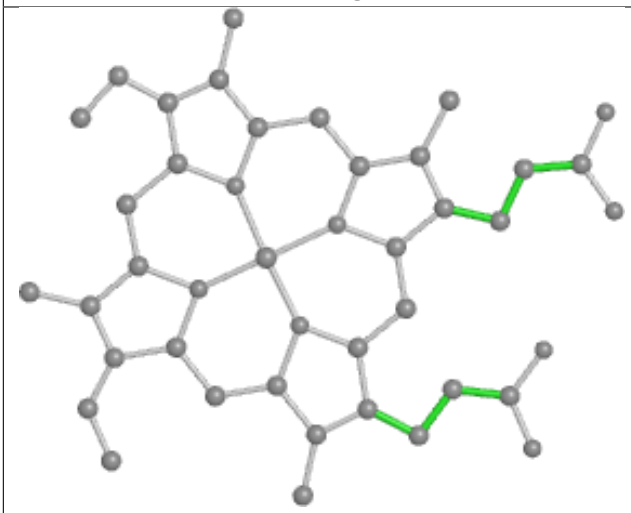


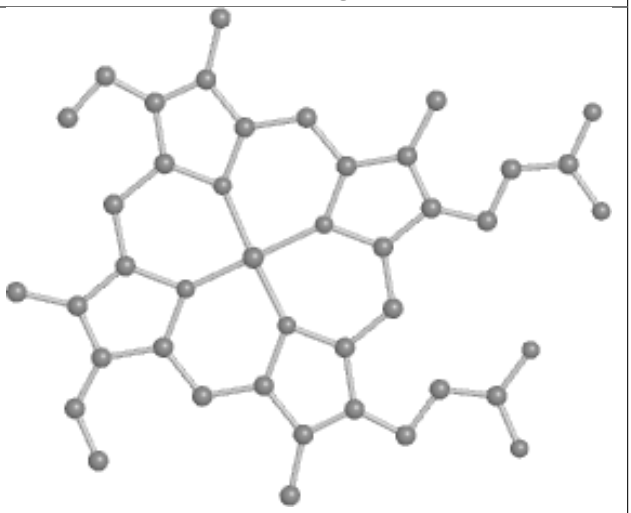
Bond lengths



Bond angles

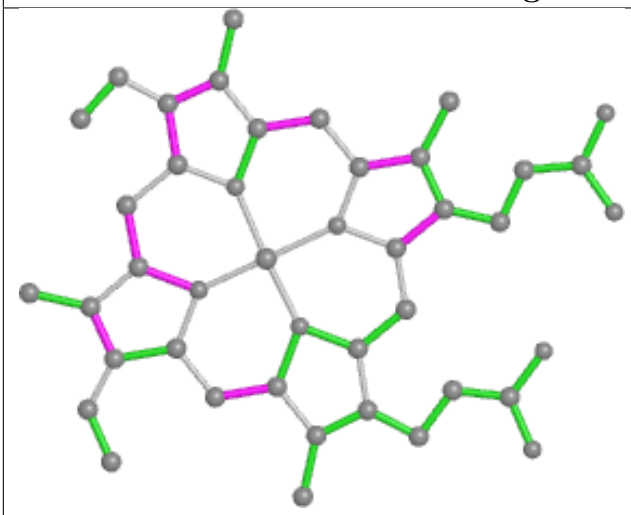


Torsions

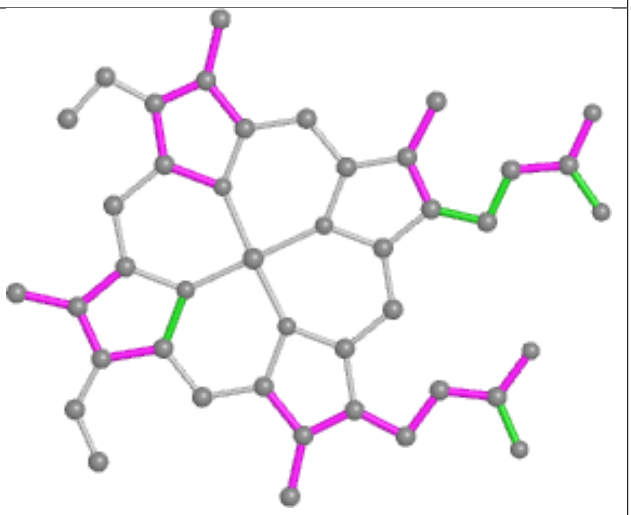


Rings

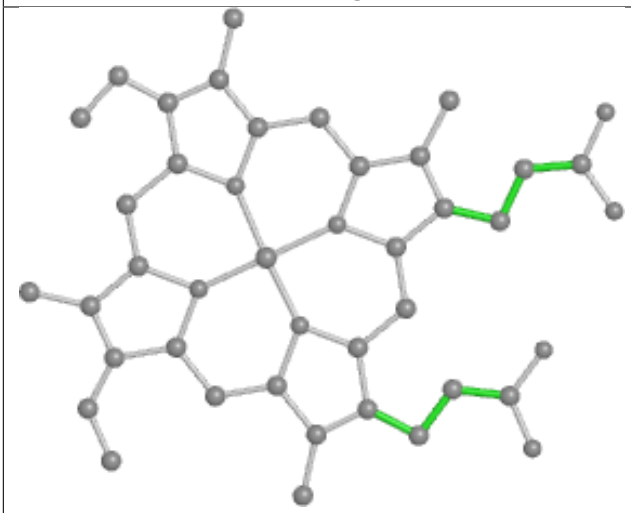
Ligand HEC B 402



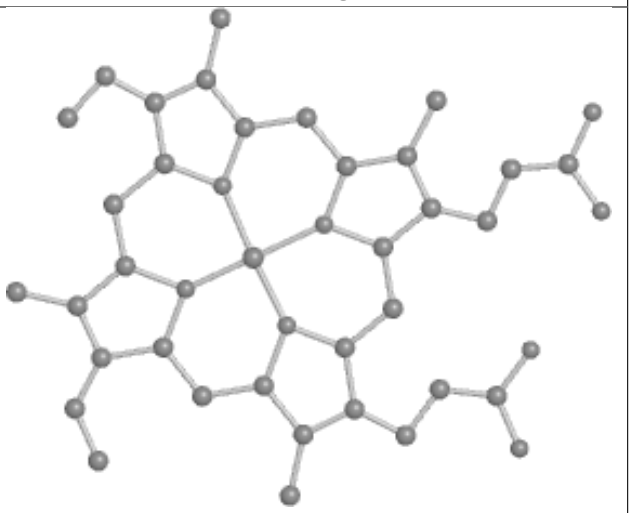
Bond lengths



Bond angles

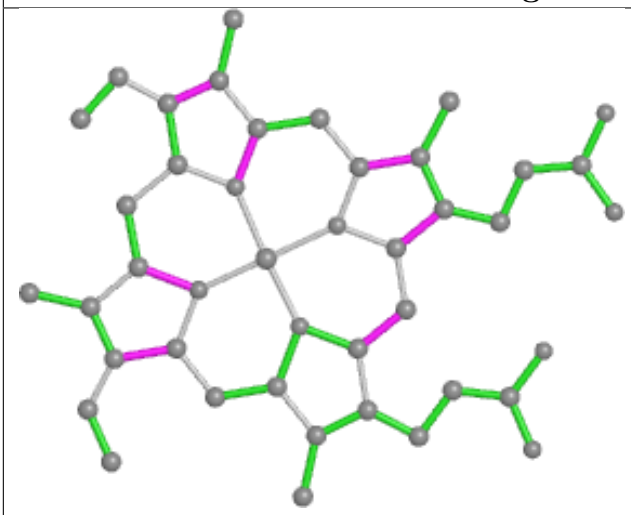


Torsions

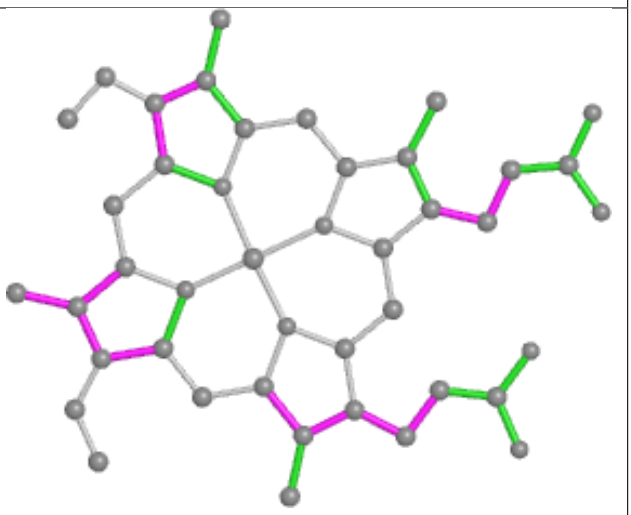


Rings

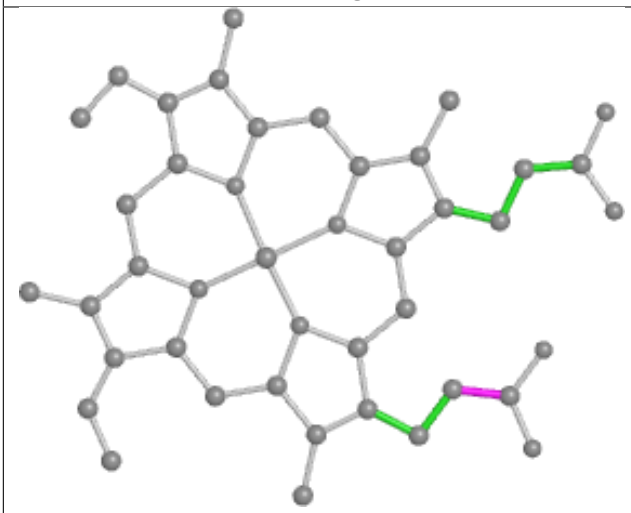
Ligand HEC A 403



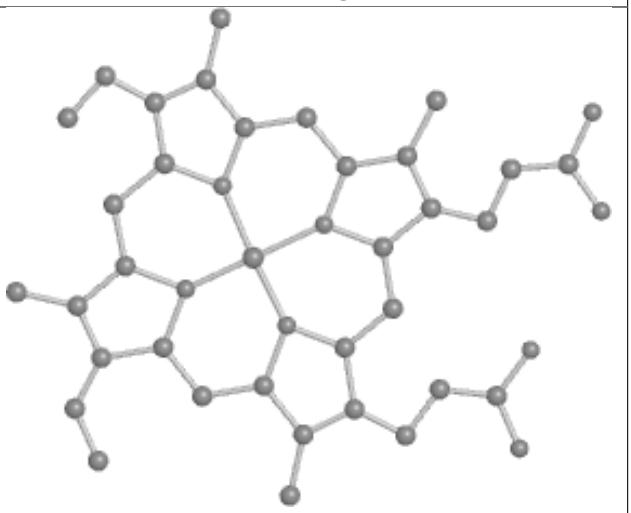
Bond lengths



Bond angles

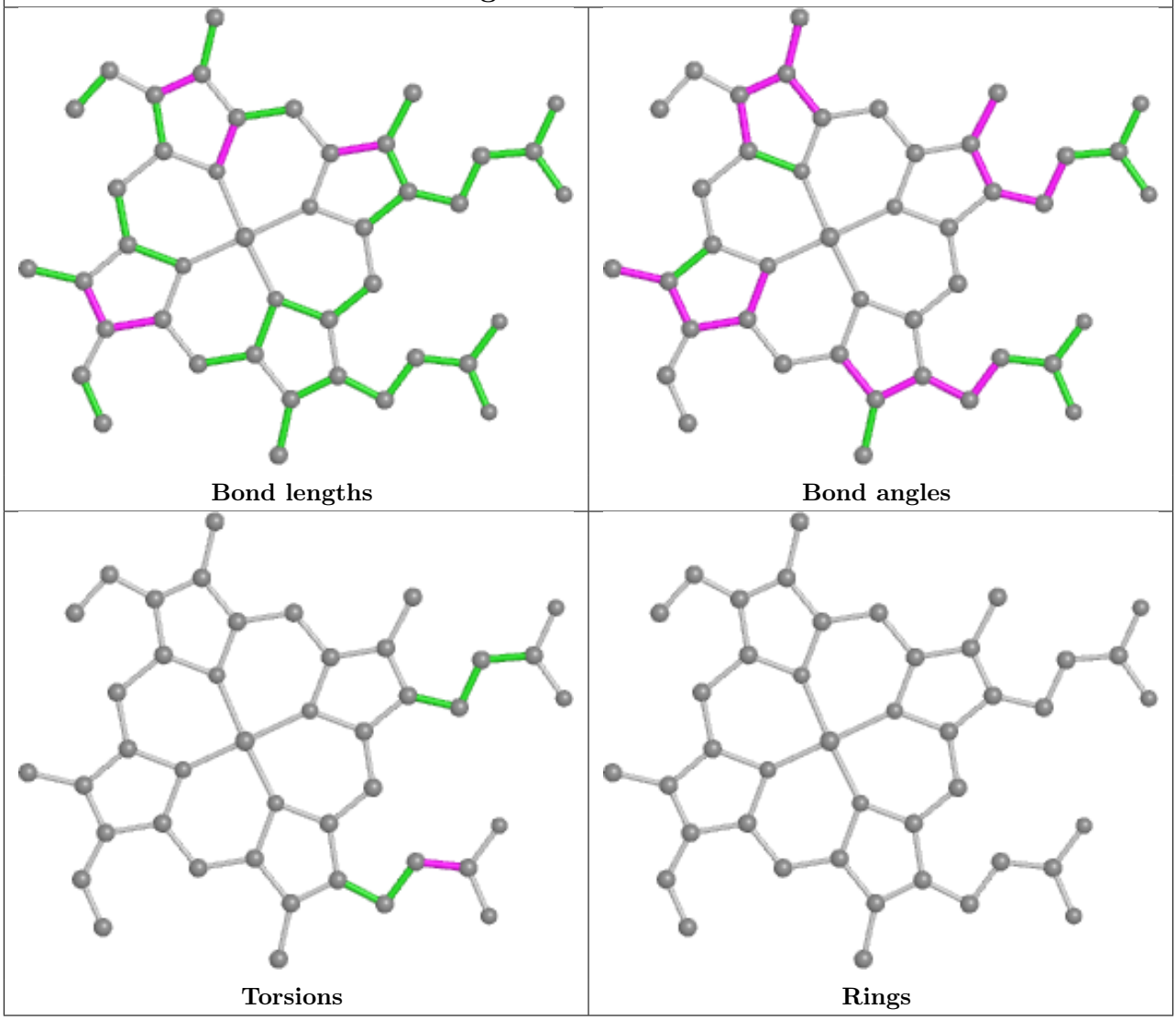


Torsions



Rings

Ligand HEC B 403



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	353/373 (94%)	-0.14	8 (2%)	60	64	29, 40, 57, 90	0
1	B	354/373 (94%)	-0.33	5 (1%)	75	78	23, 34, 53, 87	0
2	C	124/137 (90%)	-0.40	1 (0%)	86	88	25, 35, 51, 84	0
2	E	124/137 (90%)	-0.47	0	100	100	23, 28, 40, 87	0
3	D	376/385 (97%)	-0.13	10 (2%)	54	59	23, 39, 63, 84	0
3	F	376/385 (97%)	-0.39	3 (0%)	86	88	21, 29, 46, 63	0
All	All	1707/1790 (95%)	-0.27	27 (1%)	72	74	21, 35, 57, 90	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	ALA	5.0
1	B	6	ALA	4.7
1	B	7	ASP	4.7
3	D	208	THR	3.9
1	B	359	GLU	3.7
1	A	7	ASP	3.1
3	D	320	THR	3.1
2	C	7	THR	3.0
1	A	8	ASP	2.8
1	B	360	GLU	2.8
3	D	11	GLN	2.8
3	F	11[A]	GLN	2.8
3	D	260	LYS	2.7
3	D	207	GLY	2.6
3	D	386	GLY	2.6
1	A	359	GLU	2.5
1	A	302	PRO	2.5
1	B	8	ASP	2.4
3	D	379	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	243	ASP	2.2
3	D	257	GLY	2.2
3	D	209	GLU	2.2
3	D	270	GLU	2.2
3	F	29	GLY	2.1
3	F	379	VAL	2.1
1	A	269	LEU	2.1
1	A	357	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TRQ	E	57	16/17	0.93	0.16	37,42,59,77	0
2	TRQ	C	57	16/17	0.94	0.17	52,57,71,80	0
1	HYP	A	107	8/9	0.95	0.11	37,42,43,44	0
1	HYP	B	107	8/9	0.97	0.13	30,36,39,48	0

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NA	B	404	1/1	0.90	0.12	42,42,42,42	0
7	ACT	C	201	4/4	0.91	0.11	53,53,54,55	0
8	PGE	F	402	10/10	0.91	0.11	51,56,63,64	0
6	NA	A	404	1/1	0.94	0.07	47,47,47,47	0
7	ACT	F	401	4/4	0.96	0.09	40,43,48,48	0
6	NA	A	405	1/1	0.97	0.23	30,30,30,30	0

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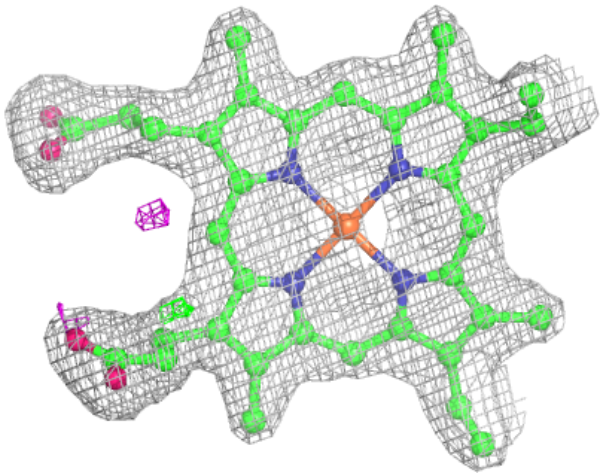
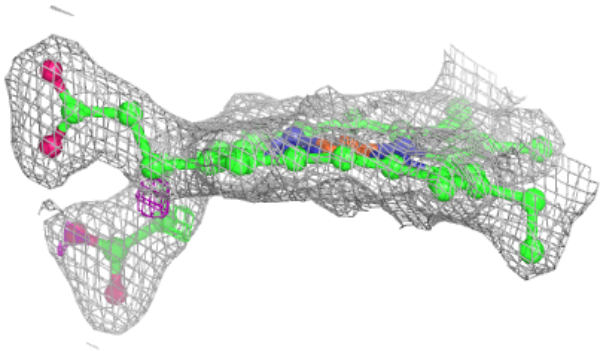
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	HEC	B	402	43/43	0.98	0.13	29,31,33,36	0
6	NA	B	405	1/1	0.98	0.18	30,30,30,30	0
5	HEC	B	403	43/43	0.98	0.14	22,25,27,28	0
5	HEC	A	402	43/43	0.98	0.13	30,34,38,42	0
5	HEC	A	403	43/43	0.98	0.17	29,32,34,40	0
4	CA	A	401	1/1	0.99	0.07	32,32,32,32	0
4	CA	B	401	1/1	1.00	0.10	26,26,26,26	0

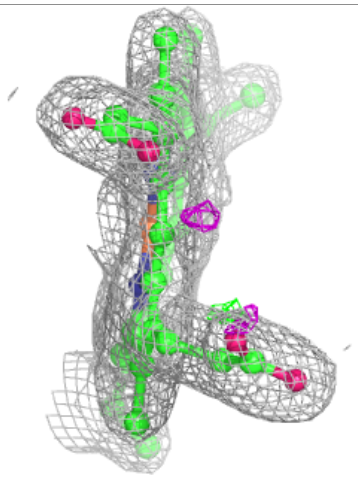
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEC B 402:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

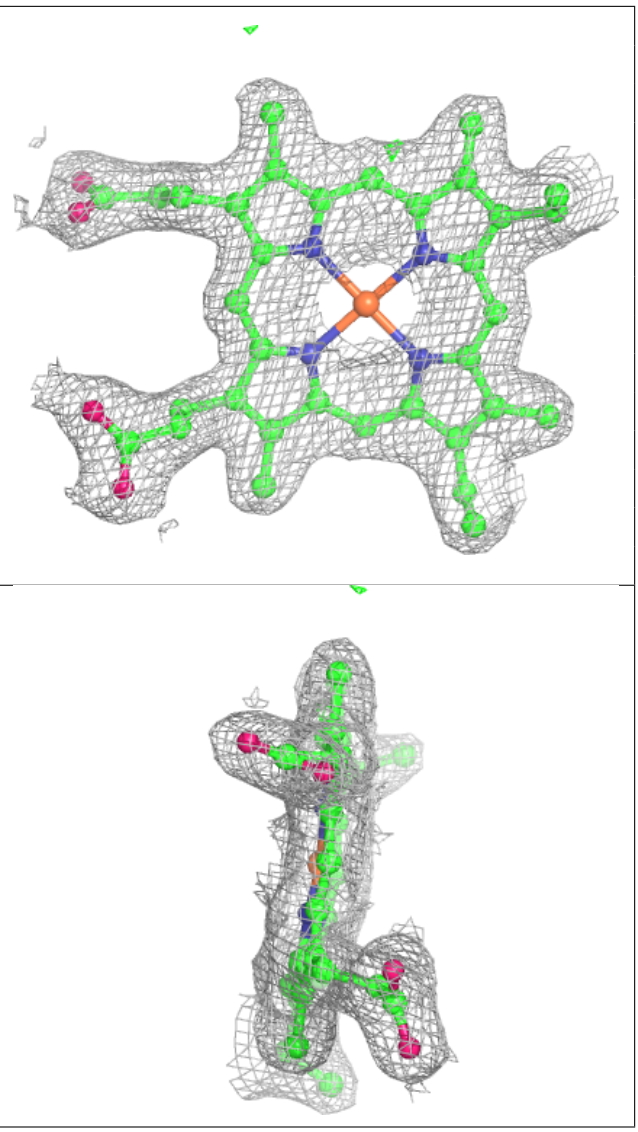






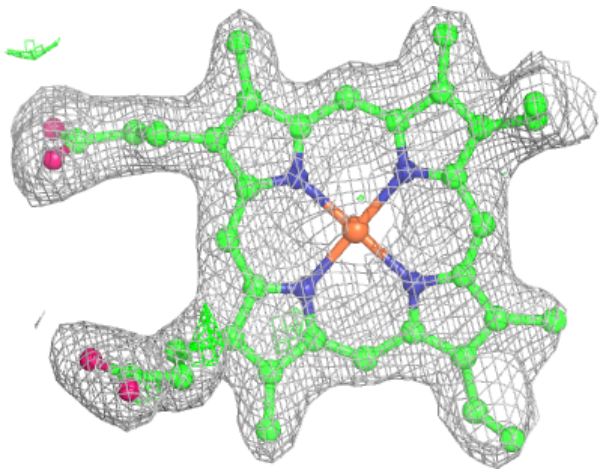
Electron density around HEC B 403:

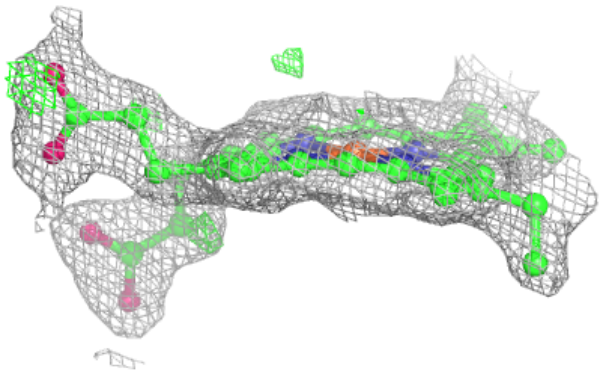
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC A 402:

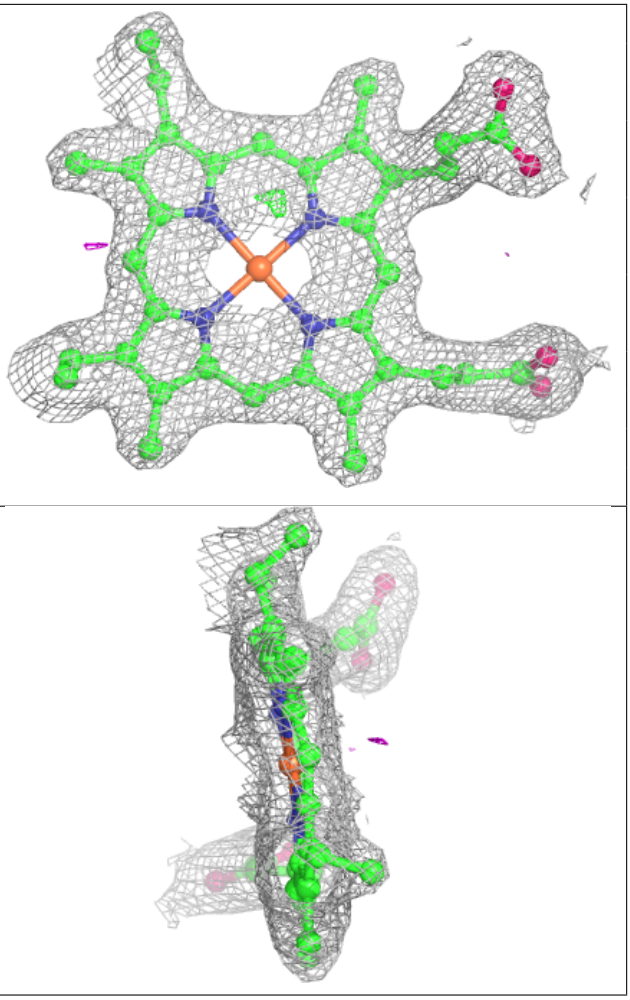
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around HEC A 403:

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



6.5 Other polymers (i)

There are no such residues in this entry.