



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 12:27 PM EST

PDB ID : 4Y5R  
Title : Crystal Structure of a T67A MauG/pre-Methylamine Dehydrogenase Complex  
Authors : Li, C.; Wilmot, C.M.  
Deposited on : 2015-02-11  
Resolution : 2.80 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](mailto: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>.

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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  
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

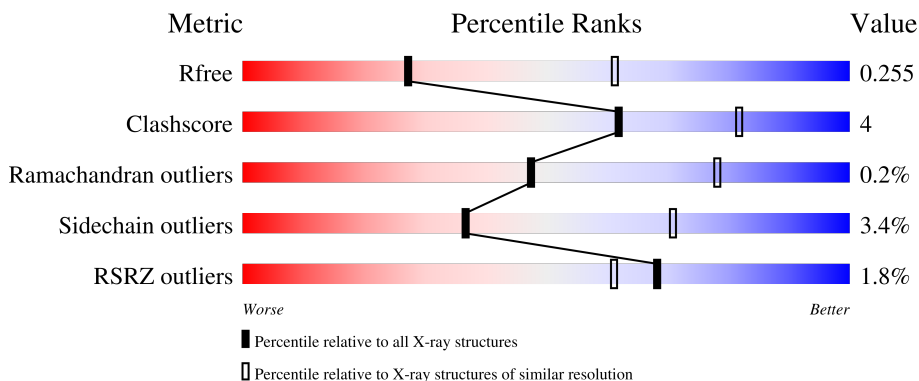
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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.



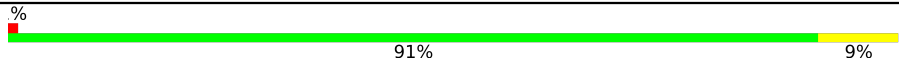
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	355	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 89%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 2px;"></div> </div> <p style="margin-left: 20px;">89% 11%</p>
1	B	355	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 90%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 2px;"></div> </div> <p style="margin-left: 20px;">90% 10%</p>
2	C	125	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 2px;"></div> </div> <p style="margin-left: 20px;">86% 14%</p>
2	E	125	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 2px;"></div> </div> <p style="margin-left: 20px;">85% 14%</p>
3	D	376	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 87%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 2px;"></div> </div> <p style="margin-left: 20px;">87% 13%</p>

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Mol	Chain	Length	Quality of chain
3	F	376	 <p>A horizontal bar chart representing the quality of the chain. The bar is 91% green and 9% yellow. A small red square is at the beginning of the bar. The percentage values '91%' and '9%' are printed below the bar.</p>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13430 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	Total	C	N	O	S	0	1	0
			2738	1710	491	526	11			
1	B	355	Total	C	N	O	S	0	0	0
			2741	1711	491	528	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	ALA	THR	engineered mutation	UNP Q51658
B	67	ALA	THR	engineered mutation	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	Total	C	N	O	S	0	1	0
			957	592	161	190	14			
2	E	125	Total	C	N	O	S	0	3	0
			963	596	161	190	16			

- 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	Total	C	N	O	S	0	1	0
			2925	1854	502	560	9			
3	F	376	Total	C	N	O	S	0	1	0
			2926	1855	502	560	9			

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

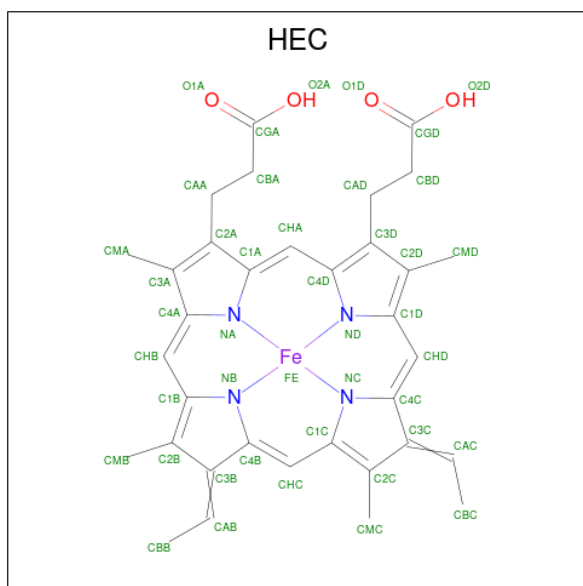
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

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

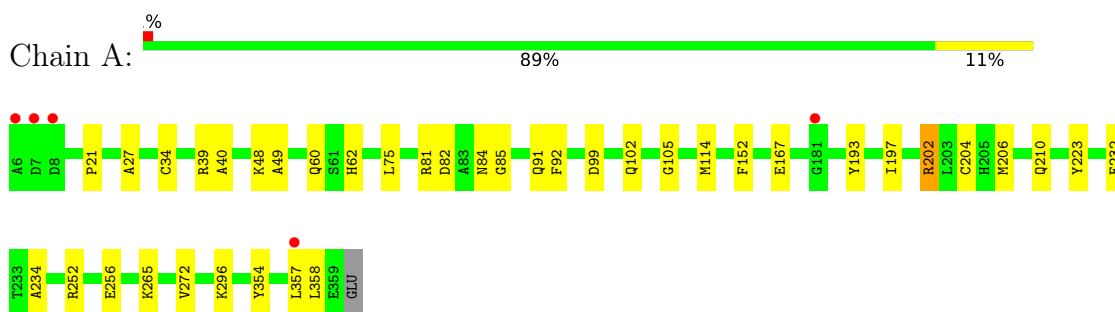
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	4	Total O 4 4	0	0
6	B	2	Total O 2 2	0	0

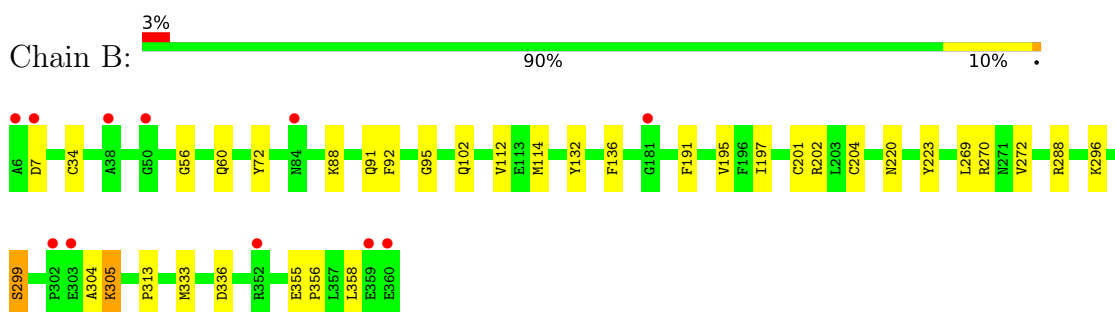
### 3 Residue-property plots [i](#)

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.

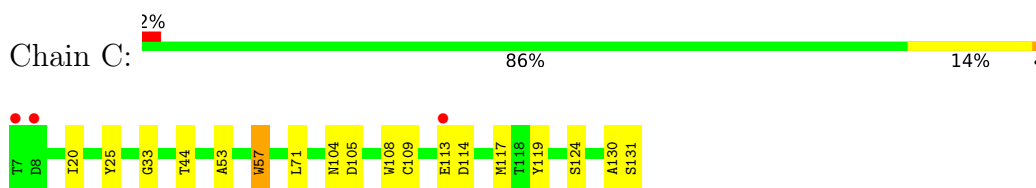
- Molecule 1: Methylamine utilization protein MauG



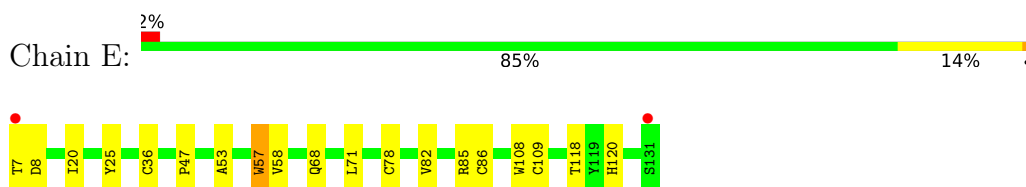
- Molecule 1: Methylamine utilization protein MauG



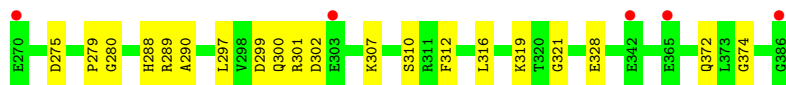
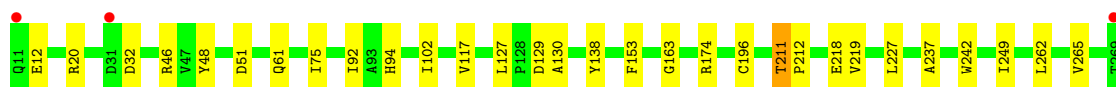
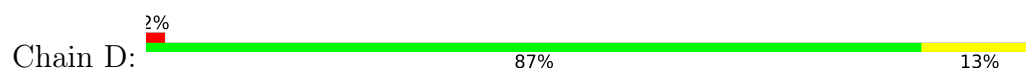
- Molecule 2: Methylamine dehydrogenase light chain



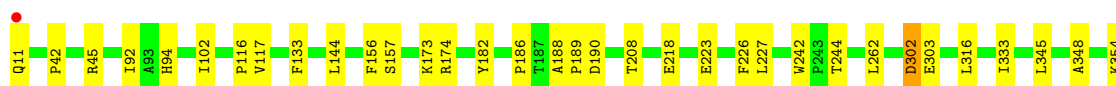
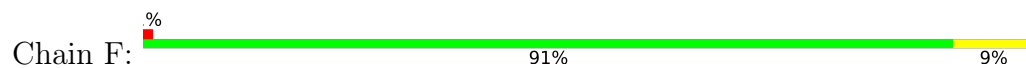
- Molecule 2: Methylamine dehydrogenase light chain



- Molecule 3: Methylamine dehydrogenase heavy chain



- Molecule 3: Methylamine dehydrogenase heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.53Å 83.52Å 107.78Å 109.94° 91.54° 105.78°	Depositor
Resolution (Å)	29.61 – 2.80 29.66 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.61-2.80) 98.3 (29.66-2.80)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 2.80Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.193 , 0.256 0.197 , 0.255	Depositor DCC
$R_{free}$ test set	2135 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.9	Xtrriage
Anisotropy	0.048	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 38.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13430	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 0AF, CA, 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	0.53	0/2805	0.71	1/3806 (0.0%)
1	B	0.55	0/2805	0.73	0/3806
2	C	0.55	0/969	0.73	0/1323
2	E	0.59	0/981	0.78	1/1340 (0.1%)
3	D	0.54	0/3006	0.72	0/4096
3	F	0.56	0/3006	0.74	0/4096
All	All	0.55	0/13572	0.73	2/18467 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	ARG	NE-CZ-NH1	5.33	122.97	120.30
2	E	8	ASP	CB-CG-OD1	5.09	122.88	118.30

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	2738	0	2616	24	0
1	B	2741	0	2614	26	0
2	C	957	0	863	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	963	0	871	16	0
3	D	2925	0	2808	27	0
3	F	2926	0	2812	13	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	86	0	62	10	0
5	B	86	0	60	13	0
6	A	4	0	0	0	0
6	B	2	0	0	0	0
All	All	13430	0	12706	115	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 4.

All (115) 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:204:CYS:SG	5:B:403:HEC:CAC	2.22	1.27
1:B:34:CYS:SG	5:B:402:HEC:CAC	2.30	1.19
1:A:204:CYS:SG	5:A:403:HEC:CAC	2.32	1.16
1:A:204:CYS:SG	5:A:403:HEC:HBC3	1.87	1.14
1:B:204:CYS:SG	5:B:403:HEC:CBC	2.37	1.12
2:C:57:0AF:HE3	2:C:108:TRP:CD1	1.85	1.11
1:B:204:CYS:SG	5:B:403:HEC:HBC3	1.91	1.11
1:A:204:CYS:SG	5:A:403:HEC:CBC	2.41	1.08
1:B:34:CYS:SG	5:B:402:HEC:HBC3	1.92	1.08
1:B:34:CYS:SG	5:B:402:HEC:CBC	2.42	1.07
2:E:57:0AF:HE3	2:E:108:TRP:CD1	1.88	1.06
2:E:57:0AF:CE3	2:E:108:TRP:CD1	2.39	1.04
2:C:57:0AF:CE3	2:C:108:TRP:CD1	2.46	0.97
2:E:57:0AF:CE3	2:E:108:TRP:HD1	1.80	0.95
1:A:34:CYS:SG	5:A:402:HEC:CAC	2.70	0.80
2:C:57:0AF:CE3	2:C:108:TRP:HD1	1.97	0.76
1:B:204:CYS:SG	5:B:403:HEC:C3C	2.75	0.75
1:A:204:CYS:SG	5:A:403:HEC:C3C	2.74	0.74
1:A:34:CYS:SG	5:A:402:HEC:HBC3	2.28	0.73
1:A:34:CYS:SG	5:A:402:HEC:CBC	2.77	0.72
1:A:114:MET:HG3	5:A:402:HEC:HMC2	1.76	0.67
1:B:34:CYS:SG	5:B:402:HEC:C3C	2.81	0.67
2:C:20:ILE:HG22	2:C:25:TYR:CZ	2.33	0.64
2:E:36[B]:CYS:SG	2:E:47:PRO:HD3	2.38	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:CYS:HG	5:B:402:HEC:HBC3	1.64	0.61
1:B:272:VAL:HG21	5:B:403:HEC:HMA3	1.83	0.59
2:C:104:ASN:OD1	3:D:307:LYS:NZ	2.36	0.58
3:F:174:ARG:HD2	3:F:208:THR:O	2.03	0.58
1:A:99:ASP:OD1	1:A:102[A]:GLN:HG2	2.05	0.57
1:B:114:MET:HG3	5:B:402:HEC:HMC2	1.87	0.57
2:E:53:ALA:HB2	2:E:109:CYS:HA	1.88	0.56
1:B:91:GLN:O	1:B:92:PHE:HB2	2.06	0.55
3:D:12:GLU:OE1	3:D:20:ARG:NH1	2.39	0.55
3:D:372:GLN:NE2	2:E:86[B]:CYS:H	2.05	0.55
1:A:48:LYS:H	1:A:62:HIS:HE1	1.53	0.55
3:D:249:ILE:HB	3:D:265:VAL:HG13	1.90	0.53
3:D:372:GLN:NE2	2:E:86[A]:CYS:H	2.06	0.53
1:A:202:ARG:HB2	1:A:206:MET:HG3	1.90	0.53
3:D:46:ARG:HD3	3:D:48:TYR:CZ	2.43	0.53
2:E:57:0AF:HE3	2:E:108:TRP:CG	2.39	0.53
2:E:78:CYS:HA	2:E:118:THR:O	2.09	0.53
3:D:288:HIS:HE1	3:D:290:ALA:HB3	1.72	0.53
1:A:21:PRO:O	1:A:27:ALA:HA	2.09	0.52
1:B:204:CYS:HG	5:B:403:HEC:HBC3	1.69	0.52
3:F:144:LEU:O	3:F:186:PRO:HG2	2.11	0.51
1:B:355:GLU:N	1:B:356:PRO:CD	2.73	0.51
1:A:60:GLN:O	1:A:62:HIS:CD2	2.64	0.50
2:E:57:0AF:CZ3	2:E:108:TRP:HD1	2.23	0.50
3:F:227:LEU:HB3	3:F:242:TRP:NE1	2.27	0.49
2:C:33:GLY:HA3	2:C:119:TYR:OH	2.13	0.49
1:B:299:SER:OG	1:B:333:MET:SD	2.70	0.49
3:F:226:PHE:O	3:F:244:THR:HA	2.12	0.49
3:D:280:GLY:HA3	3:D:301:ARG:CZ	2.42	0.49
3:D:372:GLN:HE22	2:E:86[B]:CYS:H	1.60	0.49
1:A:210:GLN:HE22	2:C:44:THR:HG21	1.78	0.49
3:D:218:GLU:HG2	3:D:219:VAL:O	2.12	0.49
3:D:297:LEU:HD22	3:D:310:SER:HB2	1.93	0.49
2:C:57:0AF:HE3	2:C:108:TRP:CG	2.43	0.49
2:E:20:ILE:HG22	2:E:25:TYR:CZ	2.48	0.48
2:C:57:0AF:CZ3	2:C:108:TRP:HD1	2.27	0.47
3:F:333:ILE:HD12	3:F:348:ALA:HB1	1.97	0.47
1:B:299:SER:HB3	1:B:304:ALA:CB	2.45	0.47
2:E:82:VAL:HA	2:E:120:HIS:HA	1.96	0.47
2:C:130:ALA:O	2:C:131:SER:HB2	2.16	0.46
1:B:72:TYR:CE2	1:B:270:ARG:HD3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:372:GLN:HE22	2:E:86[A]:CYS:H	1.63	0.46
1:B:72:TYR:CZ	1:B:270:ARG:HD3	2.51	0.46
1:A:204:CYS:HG	5:A:403:HEC:CAC	2.26	0.45
2:C:105:ASP:HB2	3:D:138:TYR:OH	2.16	0.45
3:D:61:GLN:HB3	3:D:75:ILE:HB	1.98	0.45
1:B:95:GLY:HA3	1:B:223:TYR:OH	2.17	0.45
5:B:403:HEC:CBC	5:B:403:HEC:HMC1	2.46	0.45
2:C:130:ALA:O	2:C:131:SER:CB	2.64	0.45
3:D:299:ASP:OD1	3:D:300:GLN:N	2.45	0.45
1:B:288:ARG:NH2	1:B:336:ASP:OD1	2.43	0.45
1:B:56:GLY:HA3	1:B:112:VAL:O	2.17	0.44
3:D:129:ASP:O	3:D:130:ALA:C	2.56	0.44
1:A:193:TYR:O	1:A:197:ILE:HG12	2.18	0.44
3:F:45:ARG:HG2	3:F:345:LEU:CD1	2.47	0.44
1:A:223:TYR:CE2	1:A:265:LYS:HB2	2.52	0.44
1:A:49:ALA:CB	1:A:234:ALA:HA	2.47	0.44
1:A:272:VAL:HG21	5:A:403:HEC:HMA3	1.99	0.43
1:B:191:PHE:O	1:B:195:VAL:HG23	2.18	0.43
3:F:133:PHE:CD1	3:F:156:PHE:HB2	2.53	0.43
3:F:188:ALA:HB1	3:F:189:PRO:HD2	2.00	0.43
3:D:288:HIS:CE1	3:D:290:ALA:HB3	2.52	0.43
1:A:105:GLY:HA3	1:A:152:PHE:CZ	2.53	0.43
1:B:305:LYS:O	1:B:313:PRO:HA	2.19	0.43
3:D:312:PHE:HE2	3:D:328:GLU:HG2	1.84	0.43
2:E:85:ARG:O	2:E:86[B]:CYS:HB2	2.18	0.43
1:A:91:GLN:O	1:A:92:PHE:HB2	2.18	0.42
1:B:88:LYS:HD3	1:B:220:ASN:O	2.18	0.42
3:D:211:THR:HG22	3:D:212:PRO:HD2	2.02	0.42
3:D:153:PHE:CE2	3:D:163:GLY:HA3	2.55	0.42
3:D:51:ASP:OD2	3:D:374:GLY:HA3	2.19	0.42
1:B:132:TYR:O	1:B:136:PHE:HB2	2.20	0.42
2:E:85:ARG:O	2:E:86[B]:CYS:CB	2.67	0.42
1:B:197:ILE:O	1:B:202:ARG:HD2	2.20	0.41
3:D:237:ALA:HB2	3:D:289:ARG:HG3	2.02	0.41
2:C:53:ALA:HB2	2:C:109:CYS:HA	2.02	0.41
3:D:279:PRO:HA	3:D:297:LEU:O	2.20	0.41
1:A:40:ALA:HA	1:A:354:TYR:CZ	2.56	0.41
1:A:81:ARG:CZ	1:A:85:GLY:HA2	2.50	0.41
3:F:190:ASP:OD1	3:F:190:ASP:C	2.59	0.41
2:C:109:CYS:HB2	2:C:117:MET:SD	2.61	0.41
3:D:46:ARG:HD3	3:D:48:TYR:OH	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:173:LYS:HA	3:F:173:LYS:HE2	2.02	0.41
2:C:113:GLU:O	2:C:114:ASP:HB2	2.21	0.40
3:F:42:PRO:HG3	3:F:116:PRO:HB2	2.02	0.40
3:D:227:LEU:HB3	3:D:242:TRP:NE1	2.36	0.40
3:D:265:VAL:HG21	3:D:321:GLY:HA2	2.04	0.40
1:A:82:ASP:OD1	1:A:82:ASP:C	2.60	0.40
3:F:302:ASP:OD1	3:F:303:GLU:N	2.54	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	353/355 (99%)	336 (95%)	17 (5%)	0	100	100
1	B	353/355 (99%)	334 (95%)	19 (5%)	0	100	100
2	C	123/125 (98%)	119 (97%)	4 (3%)	0	100	100
2	E	125/125 (100%)	120 (96%)	5 (4%)	0	100	100
3	D	375/376 (100%)	356 (95%)	17 (4%)	2 (0%)	29	61
3	F	375/376 (100%)	357 (95%)	17 (4%)	1 (0%)	41	72
All	All	1704/1712 (100%)	1622 (95%)	79 (5%)	3 (0%)	47	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	102	ILE
3	D	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	276/276 (100%)	266 (96%)	10 (4%)	35	69
1	B	276/276 (100%)	267 (97%)	9 (3%)	38	72
2	C	105/104 (101%)	103 (98%)	2 (2%)	57	85
2	E	107/104 (103%)	103 (96%)	4 (4%)	34	68
3	D	305/304 (100%)	294 (96%)	11 (4%)	35	69
3	F	305/304 (100%)	294 (96%)	11 (4%)	35	69
All	All	1374/1368 (100%)	1327 (97%)	47 (3%)	37	71

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	LEU
1	A	84	ASN
1	A	167	GLU
1	A	202	ARG
1	A	232	GLU
1	A	252	ARG
1	A	256	GLU
1	A	296	LYS
1	A	357	LEU
1	A	358	LEU
1	B	7	ASP
1	B	60	GLN
1	B	102	GLN
1	B	201	CYS
1	B	269	LEU
1	B	296	LYS
1	B	299	SER
1	B	305	LYS
1	B	358	LEU
2	C	71	LEU
2	C	124	SER
3	D	92	ILE

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Mol	Chain	Res	Type
3	D	94	HIS
3	D	117	VAL
3	D	127	LEU
3	D	174	ARG
3	D	211	THR
3	D	262	LEU
3	D	275	ASP
3	D	302	ASP
3	D	316	LEU
3	D	319	LYS
2	E	7	THR
2	E	58	VAL
2	E	68	GLN
2	E	71	LEU
3	F	11	GLN
3	F	92	ILE
3	F	94	HIS
3	F	117	VAL
3	F	157	SER
3	F	218	GLU
3	F	223	GLU
3	F	262	LEU
3	F	302	ASP
3	F	316	LEU
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	29	GLN
1	A	62	HIS
1	A	91	GLN
1	A	163	GLN
1	A	210	GLN
1	B	163	GLN
1	B	210	GLN
3	D	94	HIS
3	D	331	HIS
3	D	372	GLN
3	F	11	GLN
3	F	14	GLN
3	F	60	GLN

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Mol	Chain	Res	Type
3	F	300	GLN
3	F	372	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](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	0AF	E	57	2	13,16,17	1.77	2 (15%)	11,22,24	1.32	1 (9%)
2	0AF	C	57	2	13,16,17	1.74	2 (15%)	11,22,24	1.03	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	0AF	E	57	2	-	0/4/6/8	0/2/2/2
2	0AF	C	57	2	-	0/4/6/8	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	57	0AF	CZ2-CE2	5.16	1.50	1.42
2	E	57	0AF	CZ2-CE2	4.88	1.50	1.42
2	C	57	0AF	CE3-CD2	-2.29	1.37	1.42
2	E	57	0AF	CZ3-CE3	2.18	1.41	1.36



All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	57	0AF	CB-CG-CD2	2.01	129.37	126.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	57	0AF	5	0
2	C	57	0AF	5	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	403	1	32,50,50	2.04	8 (25%)	24,82,82	2.91	5 (20%)
5	HEC	B	402	1	32,50,50	2.39	10 (31%)	24,82,82	2.96	10 (41%)
5	HEC	A	402	1	32,50,50	2.22	11 (34%)	24,82,82	3.16	7 (29%)
5	HEC	B	403	1	32,50,50	2.27	8 (25%)	24,82,82	2.88	7 (29%)

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	403	1	-	2/10/54/54	-
5	HEC	B	402	1	-	1/10/54/54	-
5	HEC	A	402	1	-	1/10/54/54	-
5	HEC	B	403	1	-	0/10/54/54	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	402	HEC	C2B-C3B	7.52	1.48	1.40
5	B	403	HEC	C3C-C2C	7.22	1.48	1.40
5	B	402	HEC	C3C-C2C	7.16	1.48	1.40
5	A	402	HEC	C2B-C3B	6.90	1.48	1.40
5	B	403	HEC	C2B-C3B	6.68	1.47	1.40
5	A	403	HEC	C2B-C3B	5.88	1.46	1.40
5	A	403	HEC	C3C-C2C	5.80	1.46	1.40
5	A	402	HEC	C3C-C2C	5.60	1.46	1.40
5	B	402	HEC	C3D-C2D	3.69	1.48	1.37
5	B	402	HEC	C2A-C3A	3.38	1.47	1.37
5	B	403	HEC	C2A-C3A	3.16	1.47	1.37
5	A	402	HEC	C2A-C3A	2.89	1.46	1.37
5	A	403	HEC	C2A-C3A	2.81	1.46	1.37
5	A	402	HEC	C2A-C1A	2.74	1.48	1.42
5	A	402	HEC	C3D-C2D	2.72	1.45	1.37
5	A	402	HEC	C3A-C4A	2.63	1.48	1.42
5	A	403	HEC	C3D-C2D	2.62	1.45	1.37
5	B	403	HEC	C3D-C2D	2.61	1.45	1.37
5	B	403	HEC	C4B-C3B	2.58	1.47	1.43
5	B	402	HEC	C3A-C4A	2.51	1.48	1.42
5	A	402	HEC	C4D-CHA	2.51	1.48	1.41
5	A	403	HEC	C4B-C3B	2.50	1.47	1.43
5	B	403	HEC	C1B-CHB	2.49	1.47	1.41
5	B	402	HEC	C1D-CHD	2.38	1.47	1.41
5	A	402	HEC	C4B-C3B	2.37	1.47	1.43
5	A	403	HEC	C4D-CHA	2.36	1.47	1.41
5	A	402	HEC	C3C-C4C	2.25	1.47	1.43
5	B	402	HEC	C1C-CHC	2.24	1.47	1.41
5	B	403	HEC	C3A-C4A	2.15	1.47	1.42
5	B	402	HEC	C1B-CHB	2.14	1.46	1.41
5	A	403	HEC	C2A-C1A	2.13	1.47	1.42
5	B	403	HEC	C2A-C1A	2.11	1.47	1.42
5	A	402	HEC	C1C-CHC	2.11	1.46	1.41
5	B	402	HEC	C2A-C1A	2.09	1.47	1.42
5	A	402	HEC	C1D-CHD	2.08	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	403	HEC	C1B-CHB	2.07	1.46	1.41
5	B	402	HEC	C4B-C3B	2.03	1.46	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	402	HEC	CBD-CAD-C3D	-8.95	97.35	112.62
5	A	403	HEC	CBD-CAD-C3D	-8.31	98.43	112.62
5	A	402	HEC	C1D-C2D-C3D	-8.29	101.23	107.00
5	B	403	HEC	CBD-CAD-C3D	-7.43	99.93	112.62
5	B	403	HEC	C1D-C2D-C3D	-6.89	102.20	107.00
5	B	402	HEC	CBD-CAD-C3D	-6.84	100.94	112.62
5	B	402	HEC	CMB-C2B-C3B	6.83	133.85	125.82
5	B	402	HEC	C1D-C2D-C3D	-6.79	102.27	107.00
5	A	403	HEC	C1D-C2D-C3D	-6.78	102.28	107.00
5	B	403	HEC	CMB-C2B-C3B	6.34	133.27	125.82
5	A	402	HEC	CMB-C2B-C3B	6.25	133.17	125.82
5	A	403	HEC	CMC-C2C-C3C	5.41	132.18	125.82
5	A	403	HEC	CMB-C2B-C3B	5.02	131.73	125.82
5	B	403	HEC	CMC-C2C-C3C	4.61	131.24	125.82
5	B	402	HEC	CBA-CAA-C2A	-3.69	106.38	112.60
5	B	403	HEC	CBA-CAA-C2A	-3.64	106.47	112.60
5	B	402	HEC	CMC-C2C-C3C	3.32	129.73	125.82
5	A	402	HEC	CBA-CAA-C2A	-2.93	107.67	112.60
5	A	402	HEC	CMC-C2C-C3C	2.92	129.26	125.82
5	B	402	HEC	O2A-CGA-CBA	2.76	122.90	114.03
5	A	403	HEC	CBA-CAA-C2A	-2.70	108.05	112.60
5	A	402	HEC	C4C-C3C-C2C	-2.61	103.53	106.35
5	B	402	HEC	CMD-C2D-C3D	2.49	129.63	124.94
5	B	402	HEC	O2D-CGD-CBD	2.27	121.31	114.03
5	B	402	HEC	C4C-C3C-C2C	-2.22	103.96	106.35
5	B	402	HEC	O1A-CGA-CBA	-2.21	115.99	123.08
5	A	402	HEC	CMD-C2D-C1D	2.14	131.75	128.46
5	B	403	HEC	CMA-C3A-C2A	2.09	128.87	124.94
5	B	403	HEC	O2D-CGD-CBD	2.05	120.63	114.03

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	403	HEC	CAD-CBD-CGD-O2D
5	A	403	HEC	CAD-CBD-CGD-O1D

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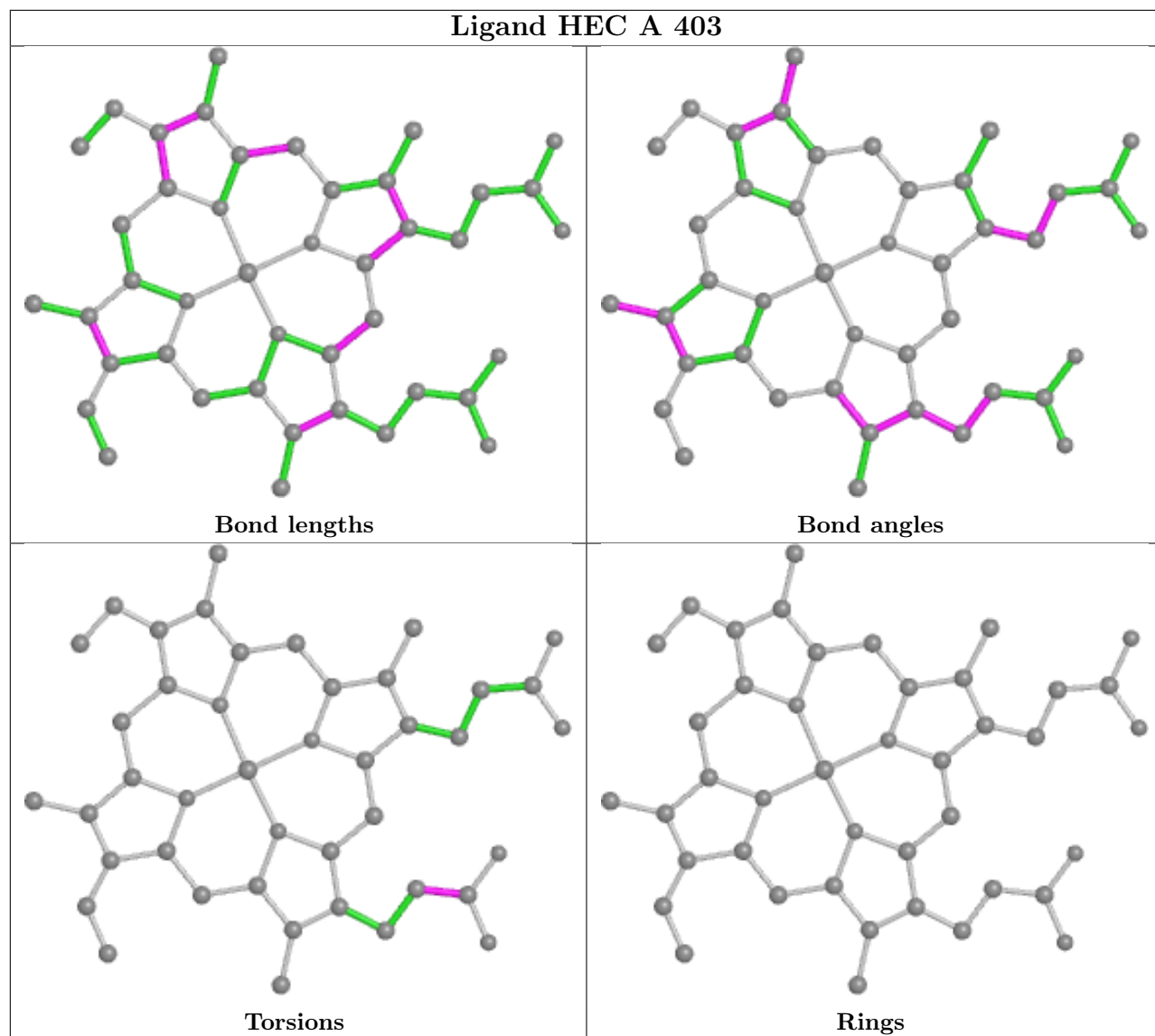
Mol	Chain	Res	Type	Atoms
5	B	402	HEC	C3D-CAD-CBD-CGD
5	A	402	HEC	CAD-CBD-CGD-O2D

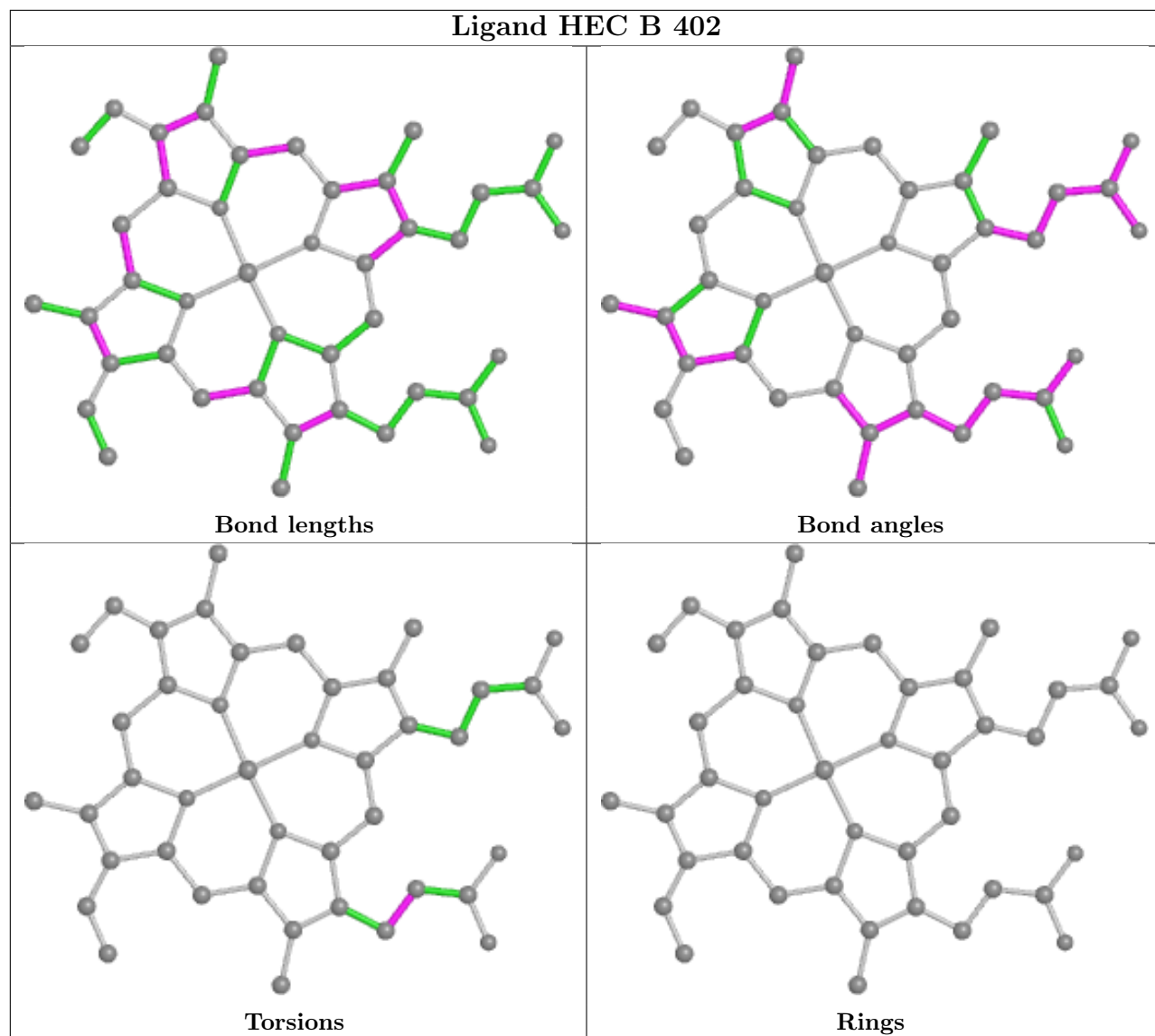
There are no ring outliers.

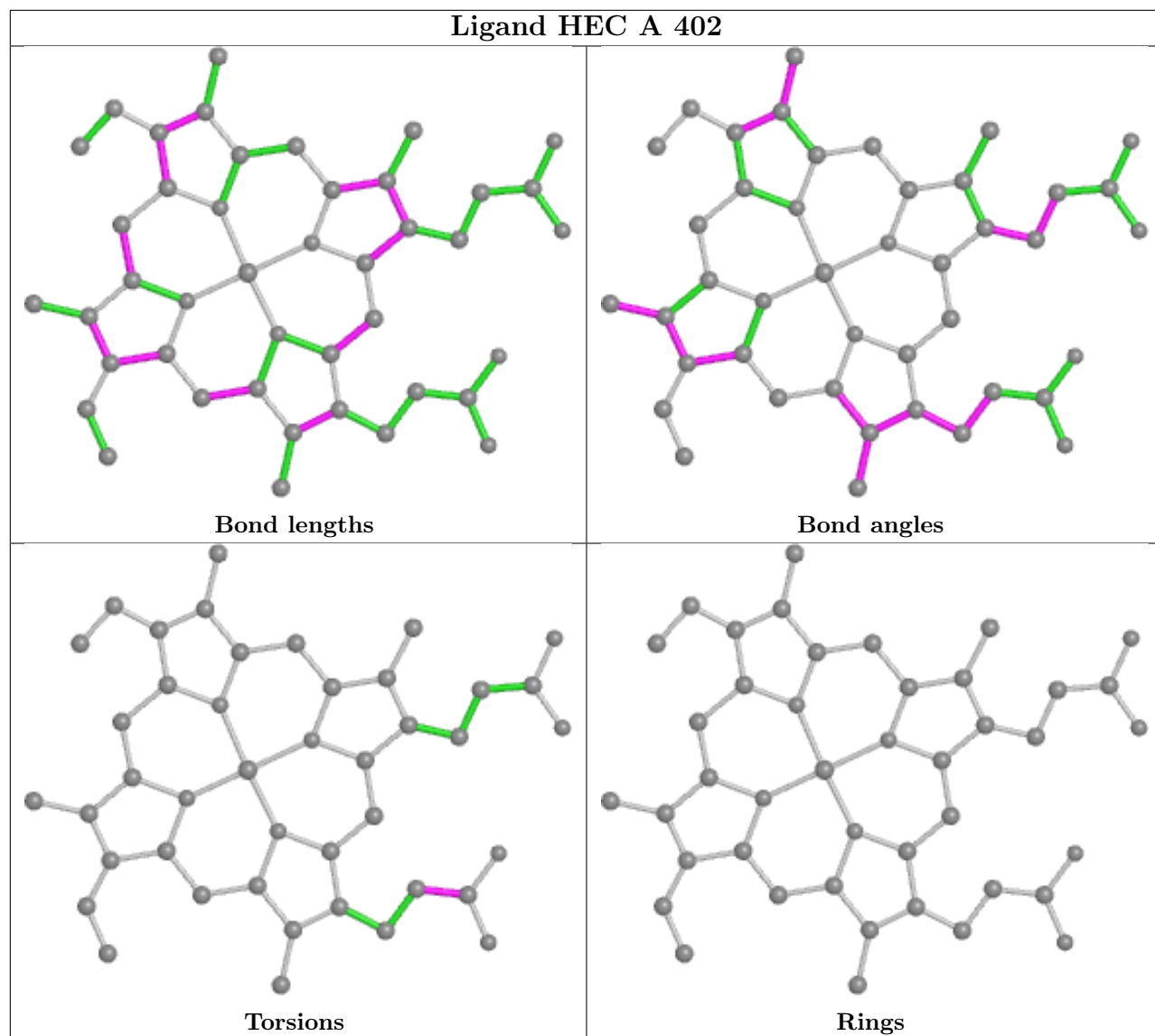
4 monomers are involved in 23 short contacts:

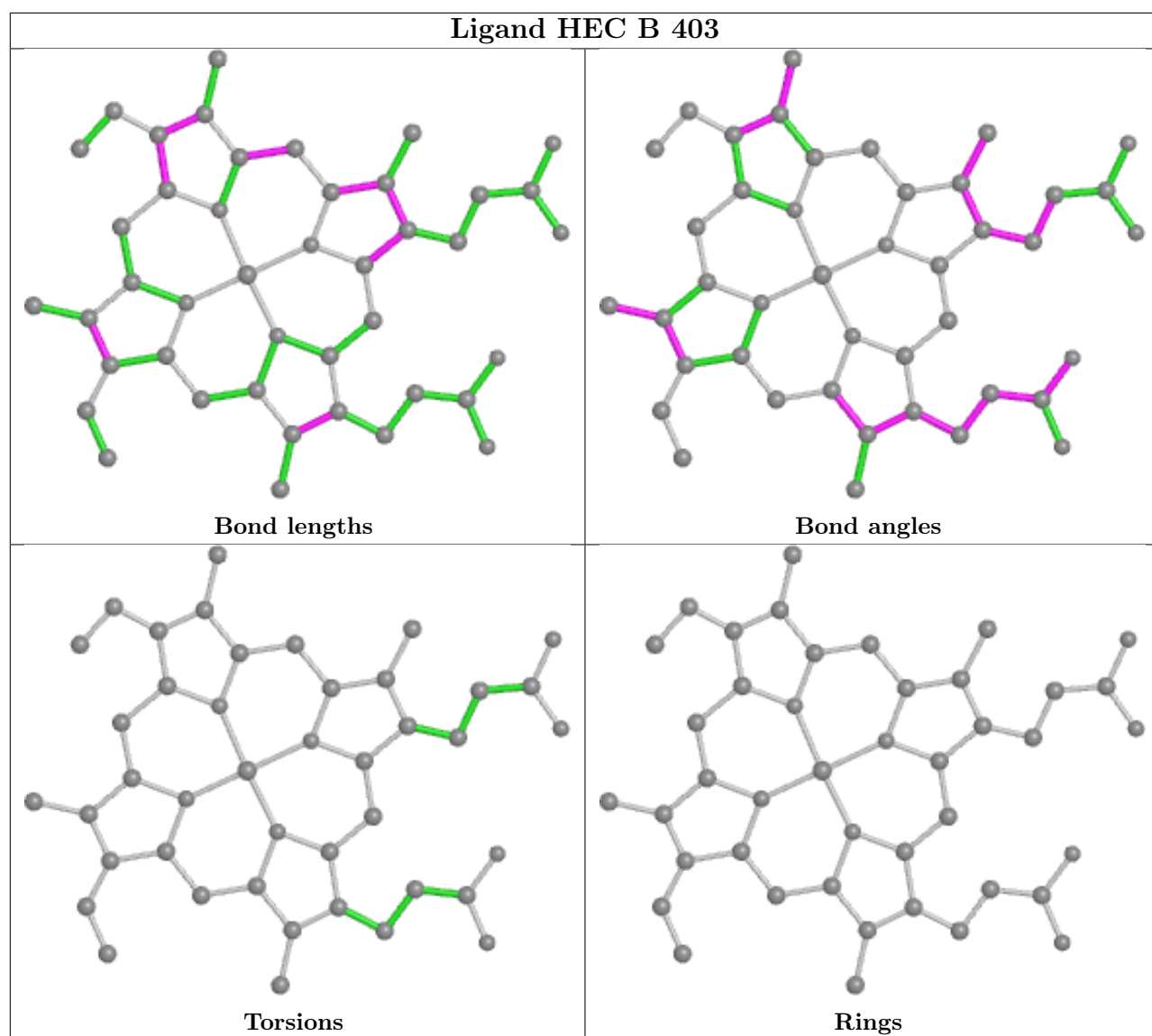
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	403	HEC	6	0
5	B	402	HEC	6	0
5	A	402	HEC	4	0
5	B	403	HEC	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	354/355 (99%)	-0.07	5 (1%) 75 70	39, 53, 73, 108	0
1	B	355/355 (100%)	-0.13	11 (3%) 49 39	35, 51, 76, 111	0
2	C	124/125 (99%)	-0.26	3 (2%) 59 49	37, 48, 67, 97	0
2	E	124/125 (99%)	-0.37	2 (1%) 72 66	31, 43, 56, 106	0
3	D	376/376 (100%)	-0.16	8 (2%) 63 54	34, 51, 78, 104	0
3	F	376/376 (100%)	-0.34	2 (0%) 91 88	30, 43, 63, 113	0
All	All	1709/1712 (99%)	-0.20	31 (1%) 68 61	30, 49, 74, 113	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	7	THR	4.9
3	D	11	GLN	4.5
3	F	11	GLN	4.3
3	D	386	GLY	4.2
1	A	7	ASP	4.1
2	E	131	SER	4.0
1	B	6	ALA	3.9
3	D	342	GLU	3.6
3	F	386	GLY	3.6
2	E	7	THR	3.1
1	B	359	GLU	3.1
1	B	360	GLU	3.0
1	B	84	ASN	3.0
3	D	269	THR	2.9
1	B	302	PRO	2.8
2	C	8	ASP	2.8
1	B	7	ASP	2.7
1	A	8	ASP	2.6
1	B	50	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
3	D	270	GLU	2.5
1	B	352	ARG	2.4
1	A	181	GLY	2.4
1	B	303	GLU	2.4
1	A	6	ALA	2.3
2	C	113	GLU	2.2
1	A	357	LEU	2.1
3	D	31	ASP	2.1
3	D	303	GLU	2.1
1	B	38	ALA	2.1
3	D	365	GLU	2.0
1	B	181	GLY	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	0AF	C	57	15/16	0.91	0.19	52,56,60,60	0
2	0AF	E	57	15/16	0.94	0.20	42,45,55,65	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, 95<sup>th</sup> 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.

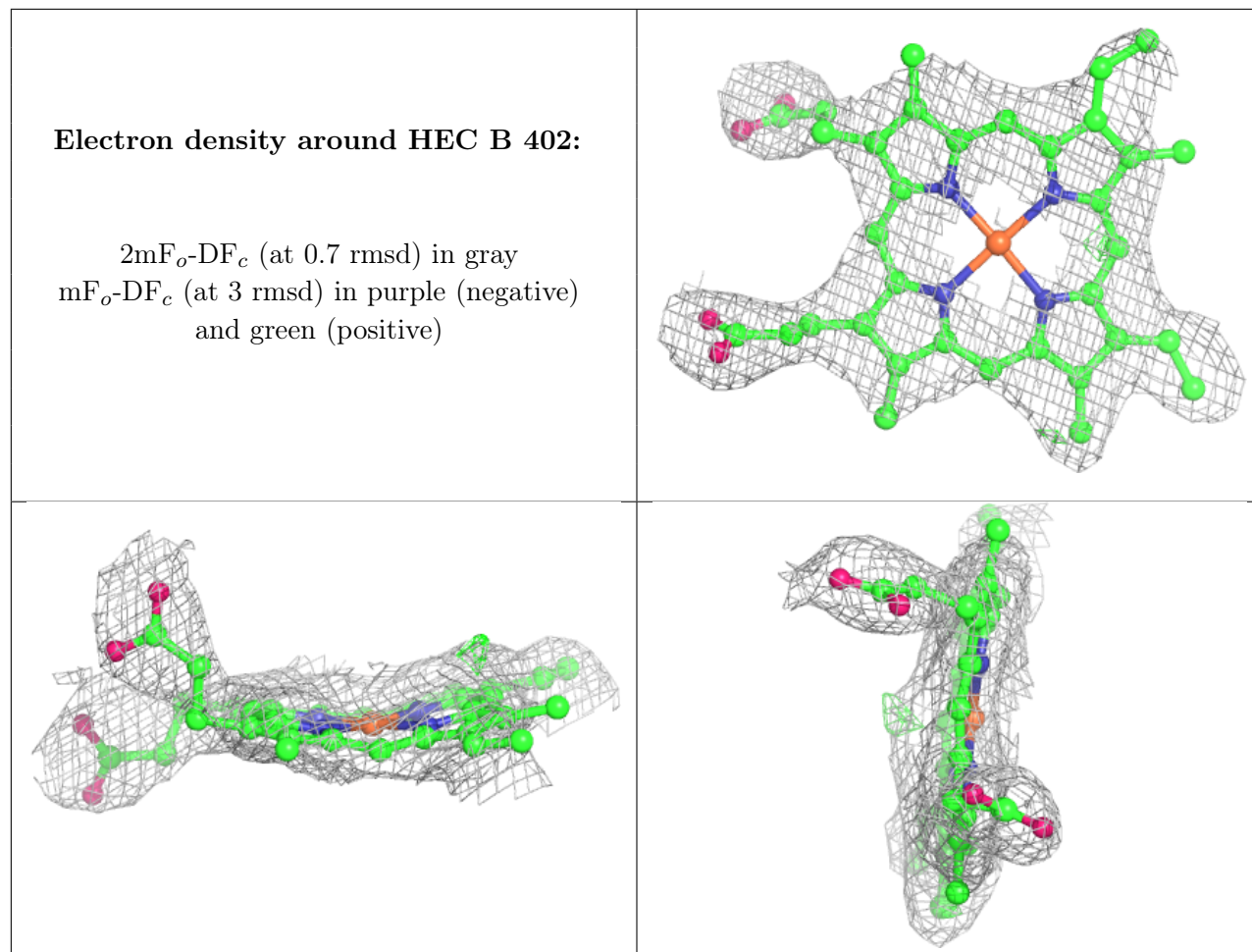
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	HEC	B	402	43/43	0.95	0.21	39,45,49,51	0
5	HEC	A	402	43/43	0.96	0.18	39,45,49,50	0
5	HEC	A	403	43/43	0.97	0.20	37,43,46,48	0
5	HEC	B	403	43/43	0.97	0.18	30,31,33,39	0

*Continued on next page...*

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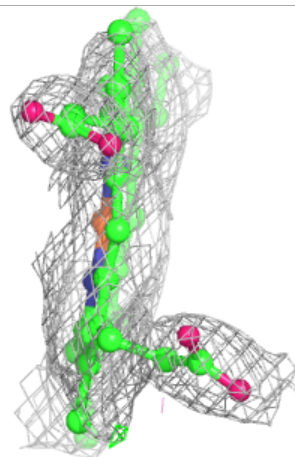
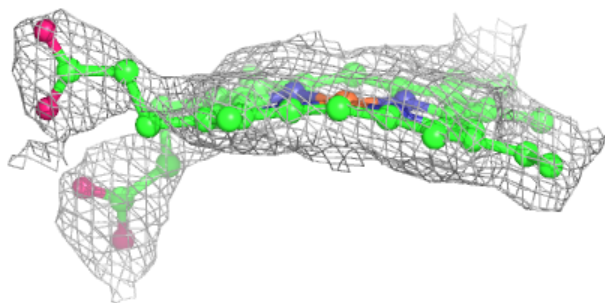
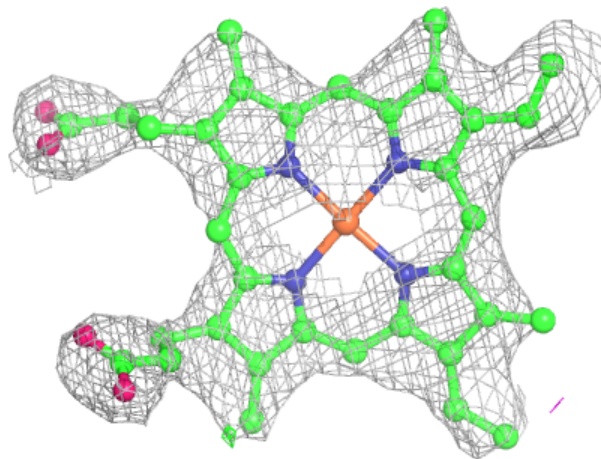
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CA	A	401	1/1	0.98	0.14	32,32,32,32	0
4	CA	B	401	1/1	0.98	0.15	40,40,40,40	0

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



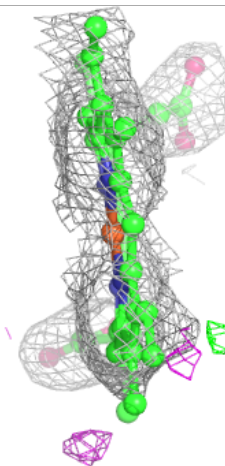
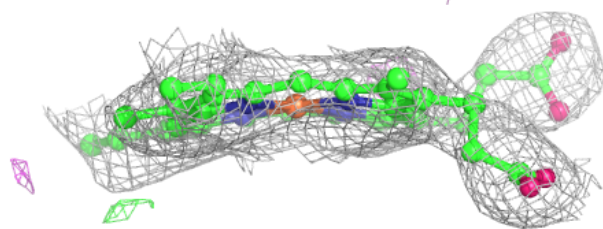
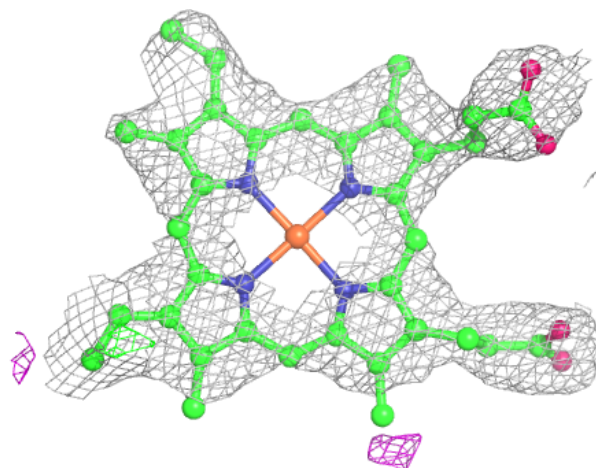
**Electron density around HEC A 402:**

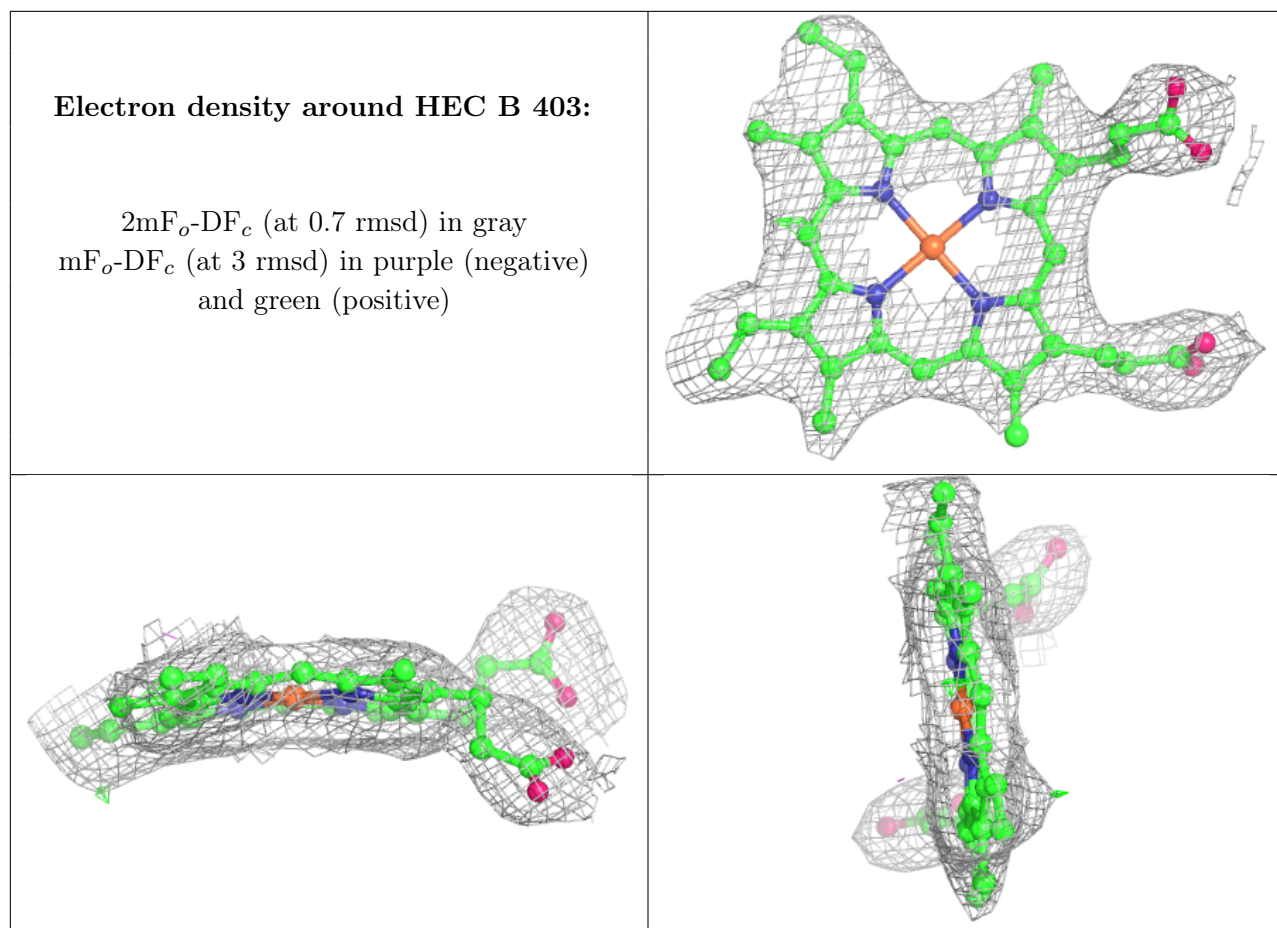
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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.