



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:27 AM UTC

PDB ID : 4FA1 / pdb_00004fa1
Title : Crystal Structure of WT MauG in Complex with Pre-Methylamine Dehydrogenase Aged 130 Days.
Authors : Yukl, E.T.; Wilmot, C.M.
Deposited on : 2012-05-21
Resolution : 2.18 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

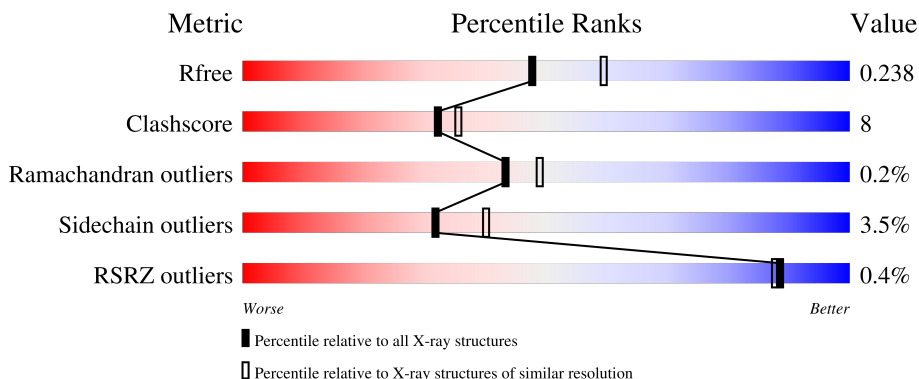
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.18 Å.

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



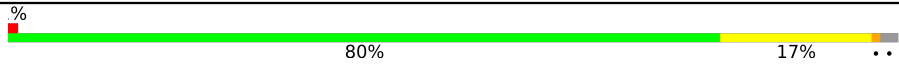
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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 $\leq 5\%$. 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	373	 75% 18% • 5%
1	B	373	 79% 16% 5%
2	C	137	 % 67% 21% • 9%
2	E	137	 % 73% 15% • 9%
3	D	385	 78% 18% ••

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Mol	Chain	Length	Quality of chain
3	F	385	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into segments: a small red segment at the start, followed by a large green segment labeled '80%', then a yellow segment labeled '17%', and finally a small grey segment at the end. A '%' symbol is positioned above the start of the bar, and two dots are positioned below the end of the bar.</p>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14647 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 2772	C 1731	N 499	O 531	S 11	0	5	0
1	B	355	Total 2809	C 1751	N 512	O 534	S 12	0	7	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	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	Total 958	C 592	N 161	O 191	S 14	0	1	0
2	E	125	Total 964	C 596	N 161	O 193	S 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 P22619
C	133	HIS	-	expression tag	UNP P22619
C	134	HIS	-	expression tag	UNP P22619
C	135	HIS	-	expression tag	UNP P22619
C	136	HIS	-	expression tag	UNP P22619
C	137	HIS	-	expression tag	UNP P22619
E	132	HIS	-	expression tag	UNP P22619
E	133	HIS	-	expression tag	UNP P22619
E	134	HIS	-	expression tag	UNP P22619
E	135	HIS	-	expression tag	UNP P22619
E	136	HIS	-	expression tag	UNP P22619
E	137	HIS	-	expression tag	UNP P22619

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	376	Total	C	N	O	S	0	4	0
			2945	1867	505	564	9			
3	F	376	Total	C	N	O	S	0	8	0
			2983	1891	514	570	8			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

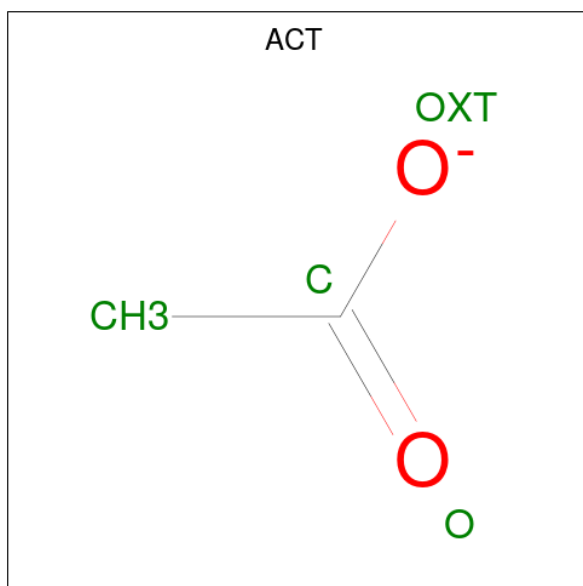
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		

- Molecule 5 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).



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

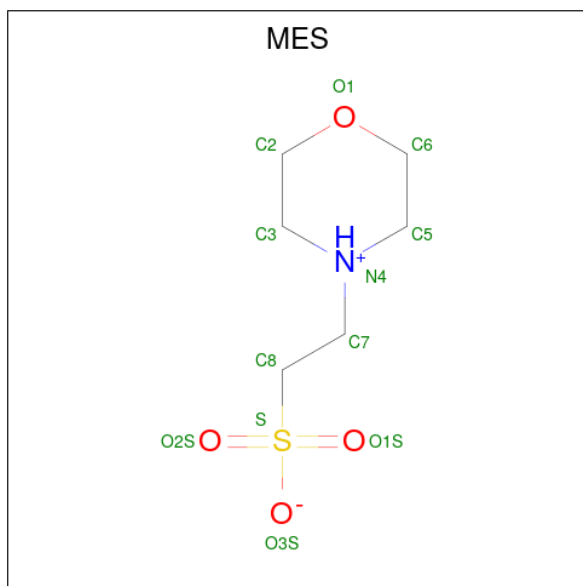
- Molecule 8 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2^-$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total	C O	0	0
			4	2 2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula:

C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
9	F	1	12	6	1	4	1	0	0


- Molecule 10 is water.

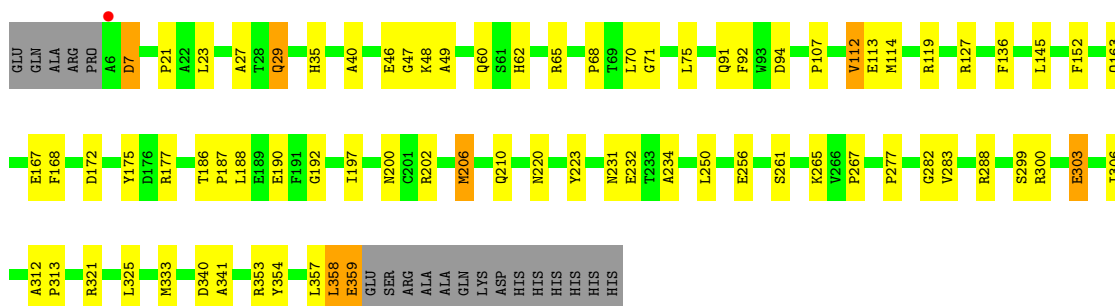
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	142	Total	O	0	2
			144	144		
10	B	230	Total	O	0	2
			232	232		
10	C	61	Total	O	0	0
			61	61		
10	D	188	Total	O	0	0
			188	188		
10	E	77	Total	O	0	0
			77	77		
10	F	313	Total	O	0	1
			314	314		

3 Residue-property plots


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.

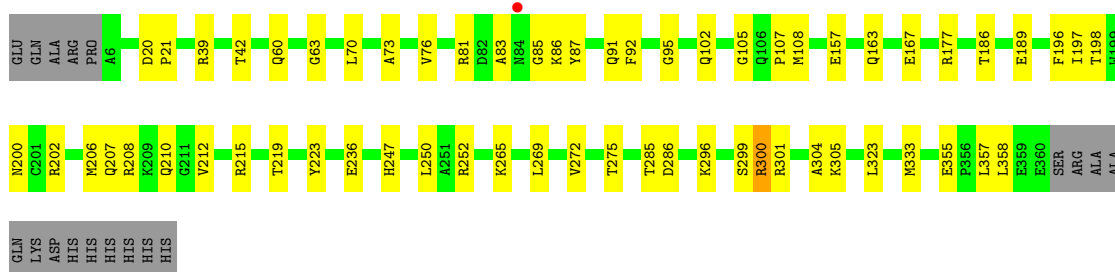
- Molecule 1: Methylamine utilization protein MauG

Chain A: 



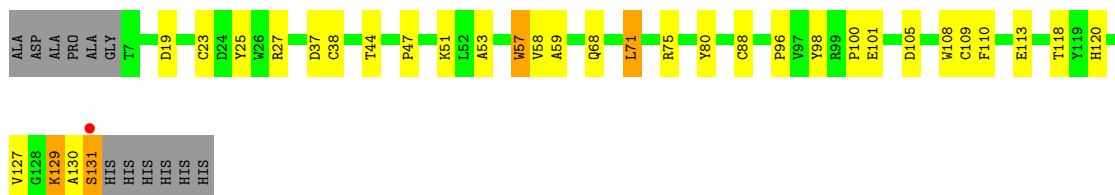
- Molecule 1: Methylamine utilization protein MauG

Chain B: 

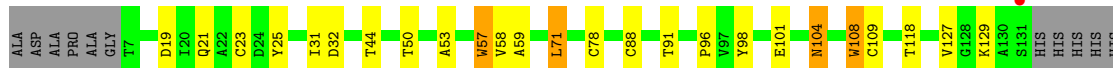
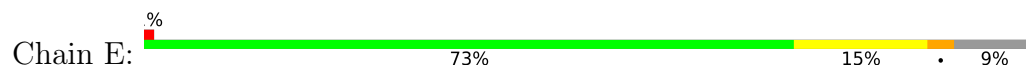


- Molecule 2: Methylamine dehydrogenase light chain

Chain C: 

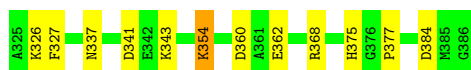
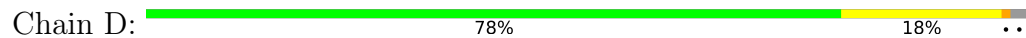


- Molecule 2: Methylamine dehydrogenase light chain

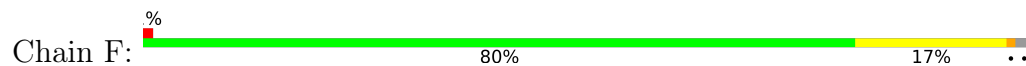


HIS

- 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, α , β , γ	55.53Å 83.52Å 107.78Å 109.94° 91.54° 105.78°	Depositor
Resolution (Å)	37.17 – 2.18 37.17 – 2.18	Depositor EDS
% Data completeness (in resolution range)	93.7 (37.17-2.18) 93.7 (37.17-2.18)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.18Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.157 , 0.227 0.171 , 0.238	Depositor DCC
R_{free} test set	4551 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtrriage
Anisotropy	0.064	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14647	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ACT, EDO, HEC, MES, CA, TRQ, NA

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	0.96	0/2845	1.06	5/3859 (0.1%)
1	B	1.10	3/2879 (0.1%)	1.12	3/3900 (0.1%)
2	C	1.06	1/969 (0.1%)	1.09	3/1323 (0.2%)
2	E	1.21	1/978 (0.1%)	1.20	1/1335 (0.1%)
3	D	1.01	0/3035	1.11	9/4134 (0.2%)
3	F	1.20	3/3075 (0.1%)	1.14	7/4185 (0.2%)
All	All	1.08	8/13781 (0.1%)	1.11	28/18736 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	131	PRO	N-CA	-7.18	1.41	1.47
2	E	108	TRP	C-N	7.05	1.43	1.33
1	B	196	PHE	N-CA	-6.12	1.39	1.46
3	F	51	ASP	N-CA	-5.99	1.40	1.46
3	F	307	LYS	N-CA	5.73	1.53	1.46
1	B	73	ALA	C-O	-5.07	1.17	1.24
2	C	37	ASP	N-CA	-5.05	1.40	1.46
1	B	207	GLN	N-CA	-5.01	1.40	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	118	THR	N-CA-C	-7.86	103.48	113.23
3	D	343	LYS	CA-C-N	7.00	127.03	119.89
3	D	343	LYS	C-N-CA	7.00	127.03	119.89
3	F	57	ALA	N-CA-C	-6.71	104.58	112.89
3	D	219	VAL	N-CA-C	-6.18	101.58	109.30
1	B	76	VAL	CA-C-N	-6.12	113.48	119.78
1	B	76	VAL	C-N-CA	-6.12	113.48	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	337	ASN	N-CA-C	-6.02	100.25	108.38
3	D	145	THR	CA-C-N	-5.96	112.72	119.28
3	D	145	THR	C-N-CA	-5.96	112.72	119.28
1	A	29	GLN	N-CA-C	5.79	118.08	108.99
2	E	104	ASN	N-CA-C	5.72	119.94	111.87
3	F	262	LEU	CA-C-N	-5.61	114.15	119.76
3	F	262	LEU	C-N-CA	-5.61	114.15	119.76
3	F	125	ILE	N-CA-C	5.52	115.54	107.37
3	F	51	ASP	CA-C-N	5.51	125.22	119.82
3	F	51	ASP	C-N-CA	5.51	125.22	119.82
1	A	127	ARG	N-CA-C	5.45	119.03	112.38
1	A	200	ASN	N-CA-C	5.34	117.85	111.71
1	A	167	GLU	N-CA-C	5.30	117.75	111.33
2	C	38	CYS	N-CA-C	5.30	119.61	113.20
1	A	325	LEU	N-CA-C	5.29	117.05	111.28
3	D	120	LEU	CA-C-N	-5.24	114.40	119.90
3	D	120	LEU	C-N-CA	-5.24	114.40	119.90
3	F	214	ILE	N-CA-C	5.19	115.33	107.75
1	B	63	GLY	N-CA-C	-5.16	104.74	112.89
2	C	47	PRO	CA-C-N	5.04	125.04	119.90
2	C	47	PRO	C-N-CA	5.04	125.04	119.90

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	2772	0	2655	54	0
1	B	2809	0	2696	44	0
2	C	958	0	862	24	0
2	E	964	0	868	22	0
3	D	2945	0	2834	46	0
3	F	2983	0	2880	44	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	86	0	60	5	0
5	B	86	0	60	4	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	B	8	0	12	2	0
8	D	4	0	3	0	0
9	F	12	0	12	0	0
10	A	144	0	0	4	0
10	B	232	0	0	9	0
10	C	61	0	0	2	0
10	D	188	0	0	6	0
10	E	77	0	0	2	0
10	F	314	0	0	8	0
All	All	14647	0	12942	212	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 8.

All (212) 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)
3:D:289[B]:ARG:HH11	3:D:289[B]:ARG:HG2	0.85	0.99
3:D:289[B]:ARG:HH11	3:D:289[B]:ARG:CG	1.76	0.98
3:D:289[B]:ARG:HG2	3:D:289[B]:ARG:NH1	1.67	0.97
1:A:299:SER:HB2	1:A:333:MET:HG3	1.48	0.95
1:A:48:LYS:H	1:A:62:HIS:HE1	1.22	0.87
3:D:121:PRO:HG3	3:F:104[A]:ARG:NH1	1.91	0.85
2:C:57:TRQ:HB2	2:C:108:TRP:NE1	1.93	0.83
1:B:198:THR:HG22	2:E:58:VAL:HG13	1.61	0.82
3:D:14:GLN:HE21	2:E:21:GLN:HE22	1.30	0.80
1:B:210:GLN:HE22	2:E:44:THR:HG21	1.47	0.79
1:A:210:GLN:HE22	2:C:44:THR:HG21	1.48	0.78
1:B:197:ILE:O	1:B:202:ARG:HD2	1.83	0.78
1:B:39[A]:ARG:HD2	10:B:710:HOH:O	1.82	0.78
1:A:197:ILE:O	1:A:202[B]:ARG:HD2	1.83	0.77
1:B:300[A]:ARG:HG3	3:F:158:PRO:HG2	1.66	0.77
3:F:11[B]:GLN:HB2	10:F:730:HOH:O	1.85	0.75
1:A:358:LEU:O	1:A:359:GLU:HB2	1.87	0.73
3:F:342:GLU:HA	10:F:794:HOH:O	1.89	0.72
1:B:198:THR:CG2	2:E:58:VAL:HG13	2.20	0.72
3:F:11[A]:GLN:NE2	3:F:11[A]:GLN:HA	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177[B]:ARG:NH2	1:B:355:GLU:OE2	2.23	0.71
2:C:71:LEU:HD13	2:C:130:ALA:HA	1.73	0.71
1:A:202[B]:ARG:HH12	2:C:127:VAL:HG11	1.54	0.71
1:B:208[A]:ARG:NH1	3:D:29:GLY:O	2.20	0.70
2:E:57:TRQ:HB2	2:E:108:TRP:NE1	2.08	0.69
1:A:197:ILE:HD13	2:C:71:LEU:HD23	1.75	0.68
1:B:86:LYS:HD2	10:B:661:HOH:O	1.94	0.67
3:D:268:LEU:HD22	3:D:277:TRP:HB3	1.77	0.67
3:F:12:GLU:OE1	3:F:20:ARG:NH1	2.29	0.66
2:E:23:CYS:SG	2:E:88[B]:CYS:HB2	2.35	0.66
1:A:70:LEU:HD13	1:A:163:GLN:NE2	2.12	0.65
1:B:39[A]:ARG:CD	10:B:710:HOH:O	2.43	0.64
1:B:198:THR:HG22	2:E:58:VAL:CG1	2.28	0.64
3:D:272:GLU:HA	10:D:665:HOH:O	1.98	0.63
1:B:215:ARG:HH22	7:B:405:EDO:H22	1.64	0.62
3:D:121:PRO:HG3	3:F:104[A]:ARG:HH12	1.62	0.62
1:A:202[B]:ARG:HH21	2:C:75:ARG:HD2	1.63	0.62
1:B:197:ILE:O	1:B:202:ARG:CD	2.48	0.62
1:A:48:LYS:H	1:A:62:HIS:CE1	2.12	0.61
1:B:107:PRO:HG3	10:B:723[A]:HOH:O	2.01	0.60
3:F:222:PRO:HG2	3:F:225:GLU:HB2	1.83	0.60
1:A:202[B]:ARG:NH1	2:C:127:VAL:HG11	2.16	0.60
3:F:82:ASN:HB3	3:F:142:THR:HB	1.84	0.59
2:C:53:ALA:HB2	2:C:109:CYS:HA	1.84	0.59
2:C:105:ASP:HB2	3:D:138:TYR:OH	2.03	0.59
1:B:200:ASN:O	5:B:403:HEC:HMC3	2.02	0.59
1:A:7:ASP:OD1	1:A:7:ASP:N	2.35	0.59
3:D:279:PRO:HB3	3:D:296:LEU:HD21	1.85	0.58
3:F:11[A]:GLN:HE21	3:F:11[A]:GLN:CA	2.16	0.58
1:A:172:ASP:O	1:A:177:ARG:NH1	2.36	0.58
1:B:197:ILE:HG22	1:B:206[B]:MET:HE1	1.86	0.58
2:E:96:PRO:HB2	2:E:98:TYR:CE1	2.39	0.58
1:A:206:MET:HA	1:A:206:MET:HE2	1.87	0.57
3:D:188:ALA:HB1	3:D:189:PRO:HD2	1.87	0.57
1:A:197:ILE:O	1:A:202[B]:ARG:NH1	2.35	0.56
2:C:101:GLU:HB2	10:C:232:HOH:O	2.05	0.56
3:F:181:CYS:C	3:F:182:TYR:CD1	2.84	0.56
1:A:60:GLN:O	1:A:62:HIS:HD2	1.89	0.56
3:D:289[A]:ARG:NH1	3:D:384:ASP:OD1	2.39	0.55
1:A:65:ARG:HH12	1:A:94:ASP:CG	2.14	0.55
2:E:101[A]:GLU:HA	10:E:274:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202[A]:ARG:HB2	1:A:206:MET:HG3	1.88	0.54
1:B:210:GLN:NE2	2:E:44:THR:HG21	2.20	0.54
1:A:119:ARG:HG2	1:A:152:PHE:CG	2.43	0.54
3:F:186:PRO:HB2	3:F:235:GLN:NE2	2.23	0.54
1:B:299:SER:HB3	1:B:304:ALA:CB	2.38	0.54
3:D:82:ASN:HB3	3:D:142:THR:HB	1.90	0.54
1:A:210:GLN:NE2	10:A:605:HOH:O	2.26	0.53
1:B:81:ARG:NH1	10:B:681:HOH:O	2.38	0.53
3:D:47:VAL:HG13	3:D:64:ILE:HB	1.91	0.53
2:C:58:VAL:HG22	2:C:59:ALA:N	2.24	0.53
1:B:198:THR:CG2	2:E:58:VAL:CG1	2.86	0.53
2:E:31:ILE:CG2	2:E:88[B]:CYS:SG	2.97	0.53
3:F:179:PRO:HD3	3:F:214:ILE:HD13	1.90	0.53
2:C:23:CYS:SG	2:C:88[B]:CYS:HB2	2.48	0.53
1:B:95:GLY:HA3	1:B:223:TYR:OH	2.08	0.53
1:B:91:GLN:O	1:B:92:PHE:HB2	2.09	0.52
3:F:331:HIS:HE1	3:F:366:GLU:OE1	1.92	0.52
1:B:212:VAL:HG11	2:E:129:LYS:HD2	1.92	0.52
1:B:285:THR:HG22	1:B:286:ASP:OD1	2.11	0.51
3:F:347:TYR:HB3	3:F:356:LEU:HD11	1.93	0.51
1:A:136:PHE:CG	1:A:145:LEU:HD21	2.46	0.51
2:C:110:PHE:CE1	3:D:157:SER:HB2	2.46	0.50
1:A:91:GLN:O	1:A:92:PHE:HB2	2.11	0.50
1:A:250:LEU:HD22	1:A:261:SER:HB2	1.93	0.50
1:B:81:ARG:NH1	10:B:707:HOH:O	2.37	0.50
1:A:113:GLU:HG2	5:A:402:HEC:HBC2	1.92	0.50
3:D:54:HIS:HD2	10:D:677:HOH:O	1.94	0.50
3:D:277:TRP:CE2	3:D:300:GLN:HG3	2.47	0.49
1:A:288:ARG:NH1	1:A:340:ASP:OD1	2.44	0.49
3:D:362:GLU:HA	3:D:362:GLU:OE1	2.12	0.49
3:F:45:ARG:NH2	3:F:343:LYS:O	2.45	0.49
1:A:70:LEU:HD13	1:A:163:GLN:HE21	1.76	0.49
1:A:312:ALA:HB1	1:A:313:PRO:HD2	1.95	0.48
3:D:236:LYS:NZ	3:D:384:ASP:O	2.44	0.48
3:F:174:ARG:NH2	3:F:207:GLY:O	2.41	0.48
1:A:21:PRO:O	1:A:27:ALA:HA	2.13	0.48
2:C:57:TRQ:HB2	2:C:108:TRP:HE1	1.73	0.48
3:F:205:ALA:HB3	3:F:213:GLU:HB3	1.95	0.48
3:D:275:ASP:HB2	10:D:665:HOH:O	2.13	0.48
10:B:706:HOH:O	2:E:127:VAL:HG12	2.13	0.48
1:A:40:ALA:HA	1:A:354:TYR:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:92:ILE:HG12	3:D:114:PHE:HB2	1.96	0.48
1:A:48:LYS:N	1:A:62:HIS:HE1	2.01	0.48
3:D:51:ASP:HA	3:D:377:PRO:HA	1.96	0.48
1:B:215:ARG:HH22	7:B:405:EDO:C2	2.26	0.47
1:B:202:ARG:HB2	1:B:206[B]:MET:HE2	1.96	0.47
2:C:51:LYS:HD2	2:C:113:GLU:HB3	1.96	0.47
3:F:42:PRO:HG3	3:F:116:PRO:HB2	1.96	0.47
3:F:115:ASP:O	3:F:119:LEU:HA	2.13	0.47
1:A:277:PRO:HB2	1:A:282:GLY:O	2.15	0.47
1:B:299:SER:HB2	1:B:333:MET:HG3	1.96	0.47
3:F:365[A]:GLU:OE1	10:F:738:HOH:O	2.20	0.47
3:D:269:THR:OG1	3:D:272:GLU:HB2	2.15	0.47
3:F:11[A]:GLN:HA	3:F:11[A]:GLN:HE21	1.75	0.47
1:A:223:TYR:CE2	1:A:265:LYS:HB2	2.49	0.47
2:C:19:ASP:O	2:C:25:TYR:HB2	2.14	0.47
3:F:199:GLY:HA3	3:F:219:VAL:HG13	1.97	0.47
1:B:42:THR:HG21	1:B:275:THR:HB	1.97	0.46
1:A:312:ALA:HB1	1:A:313:PRO:CD	2.45	0.46
1:B:247:HIS:HB3	1:B:250:LEU:HB3	1.98	0.46
3:F:343:LYS:N	3:F:344:PRO:CD	2.78	0.46
2:C:68:GLN:HB3	2:C:129:LYS:HE3	1.98	0.46
3:F:269:THR:OG1	3:F:272:GLU:HG3	2.16	0.46
1:A:46[A]:GLU:HG3	1:A:47:GLY:N	2.30	0.46
1:A:48:LYS:HB2	1:A:62:HIS:CE1	2.51	0.46
3:F:104[B]:ARG:HD3	10:F:530:HOH:O	2.15	0.46
3:D:315:VAL:O	3:D:324:LEU:N	2.44	0.46
3:D:368:ARG:HA	10:D:625:HOH:O	2.15	0.46
1:A:192:GLY:HA3	1:A:341:ALA:O	2.17	0.45
5:B:402:HEC:HBB3	5:B:402:HEC:CMB	2.47	0.45
3:D:252:ILE:HD12	3:D:252:ILE:N	2.31	0.45
2:C:25:TYR:CE2	2:C:27:ARG:HB2	2.51	0.45
1:B:223:TYR:CZ	1:B:265:LYS:HB2	2.51	0.45
3:D:140:TRP:CE2	3:D:233:TYR:HB3	2.52	0.45
1:B:223:TYR:CE2	1:B:265:LYS:HB2	2.51	0.45
2:E:101[B]:GLU:HA	10:E:274:HOH:O	2.17	0.45
3:F:147:ASP:OD1	3:F:147:ASP:C	2.59	0.45
2:E:91:THR:HB	3:F:306:HIS:CE1	2.51	0.45
1:B:252:ARG:HD3	10:B:636:HOH:O	2.17	0.45
1:B:305:LYS:NZ	10:B:638:HOH:O	2.48	0.45
1:A:353:ARG:NE	10:A:583:HOH:O	2.49	0.44
3:F:349:LEU:HD21	3:F:377:PRO:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:PRO:HG2	5:A:402:HEC:HBA1	1.99	0.44
2:C:57:TRQ:HB2	2:C:108:TRP:CE2	2.52	0.44
3:D:186:PRO:HB2	3:D:235:GLN:NE2	2.32	0.44
1:A:175:TYR:CD2	1:A:175:TYR:C	2.95	0.44
1:B:301:ARG:NH2	3:F:177[B]:ASP:OD1	2.50	0.44
3:D:289[B]:ARG:CG	3:D:289[B]:ARG:NH1	2.49	0.44
1:A:197:ILE:HA	1:A:202[A]:ARG:HB3	2.00	0.44
3:F:280:GLY:HA3	3:F:301:ARG:CZ	2.48	0.44
1:B:186:THR:OG1	1:B:189:GLU:HG3	2.18	0.44
2:E:53:ALA:HB2	2:E:109:CYS:HA	1.99	0.44
3:F:288:HIS:HE1	3:F:290:ALA:HB3	1.83	0.44
1:A:35:HIS:CE1	1:A:70:LEU:HD21	2.53	0.44
1:A:71:GLY:HA2	1:A:168:PHE:O	2.17	0.44
3:F:288:HIS:CE1	3:F:290:ALA:HB3	2.53	0.43
3:F:130:ALA:N	3:F:131:PRO:HD3	2.32	0.43
1:A:29:GLN:HE22	5:A:402:HEC:HBC3	1.83	0.43
2:C:80:TYR:HB2	2:C:120:HIS:HB2	2.00	0.43
3:D:188:ALA:HB1	3:D:189:PRO:CD	2.49	0.43
3:D:314:VAL:HG12	3:D:326:LYS:HG3	2.00	0.43
2:C:96:PRO:HB2	2:C:98:TYR:CE1	2.53	0.43
1:B:83:ALA:C	1:B:85:GLY:H	2.26	0.43
1:B:70:LEU:HD22	5:B:402:HEC:HMA2	2.00	0.43
2:C:131:SER:HA	10:C:255:HOH:O	2.19	0.43
3:D:312:PHE:HA	3:D:327:PHE:O	2.19	0.43
3:F:333:ILE:HD12	3:F:348:ALA:HB1	2.00	0.43
2:E:32:ASP:OD2	2:E:104:ASN:O	2.37	0.43
1:A:40:ALA:HA	1:A:354:TYR:CE1	2.53	0.43
2:C:118:THR:HG23	3:D:99:PHE:CE1	2.54	0.42
3:D:43:ASP:HB2	10:D:639:HOH:O	2.17	0.42
1:A:188:LEU:HG	1:A:341:ALA:HA	2.01	0.42
1:A:267:PRO:HD3	5:A:403:HEC:CAD	2.48	0.42
3:D:42:PRO:HD3	3:D:117:VAL:HG12	2.01	0.42
3:D:285:VAL:HA	3:D:295:TYR:O	2.19	0.42
3:F:260[A]:LYS:HE3	3:F:262:LEU:CD1	2.49	0.42
1:A:112[A]:VAL:HG22	10:A:613:HOH:O	2.19	0.42
1:A:206:MET:O	1:A:220:ASN:HB3	2.19	0.42
3:D:341:ASP:N	3:D:341:ASP:OD1	2.49	0.42
3:D:40:PRO:O	3:D:41:ALA:C	2.62	0.42
1:B:20:ASP:HA	1:B:21:PRO:HD2	1.92	0.42
1:A:114:MET:HG3	5:A:402:HEC:HMC2	2.01	0.42
3:F:50:ASN:HB3	10:F:536:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:251:GLN:O	3:F:262:LEU:HB2	2.20	0.42
1:A:49:ALA:CB	1:A:234:ALA:HA	2.50	0.41
2:E:78:CYS:HA	2:E:118:THR:O	2.20	0.41
3:F:173[A]:LYS:HE2	10:F:692:HOH:O	2.20	0.41
1:B:81:ARG:HB2	1:B:87:TYR:CE2	2.55	0.41
3:D:289[B]:ARG:HD3	3:D:384:ASP:OD2	2.20	0.41
3:D:360:ASP:OD2	3:D:360:ASP:C	2.64	0.41
2:E:19:ASP:O	2:E:25:TYR:HB2	2.20	0.41
3:F:51:ASP:HA	3:F:377:PRO:HA	2.02	0.41
3:F:104[B]:ARG:NH1	10:F:520:HOH:O	2.38	0.41
3:F:107:ARG:NE	3:F:130:ALA:HB1	2.35	0.41
3:D:354:LYS:HE2	3:D:375:HIS:O	2.20	0.41
1:A:107:PRO:HG3	10:A:638[A]:HOH:O	2.20	0.41
2:C:98:TYR:C	2:C:100:PRO:HD3	2.45	0.41
3:F:360:ASP:HB2	3:F:367:LEU:HD11	2.01	0.41
1:B:105:GLY:O	1:B:108:MET:HB2	2.21	0.41
1:B:272:VAL:HG21	5:B:403:HEC:HMA3	2.02	0.41
3:D:36:ILE:HD12	2:E:50:THR:O	2.21	0.41
3:D:155:GLN:NE2	10:D:666:HOH:O	2.50	0.41
1:A:303:GLU:H	1:A:303:GLU:HG3	1.33	0.41
3:D:292:ASP:OD2	3:D:319:LYS:HD3	2.21	0.41
2:E:59:ALA:O	2:E:71:LEU:HA	2.21	0.41
1:B:70:LEU:HD13	1:B:163:GLN:NE2	2.35	0.40
3:F:88:ASP:HA	10:F:676:HOH:O	2.20	0.40
1:B:296:LYS:O	1:B:305:LYS:HE3	2.21	0.40
1:A:231:ASN:ND2	1:A:283:VAL:HA	2.36	0.40
3:D:91:PHE:CD1	3:D:113:VAL:HG13	2.56	0.40
1:A:186:THR:O	1:A:187:PRO:C	2.62	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	357/373 (96%)	345 (97%)	12 (3%)	0	100	100
1	B	360/373 (96%)	351 (98%)	9 (2%)	0	100	100
2	C	123/137 (90%)	119 (97%)	4 (3%)	0	100	100
2	E	124/137 (90%)	116 (94%)	8 (6%)	0	100	100
3	D	378/385 (98%)	358 (95%)	17 (4%)	3 (1%)	16	14
3	F	381/385 (99%)	367 (96%)	13 (3%)	1 (0%)	36	39
All	All	1723/1790 (96%)	1656 (96%)	63 (4%)	4 (0%)	43	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	207	GLY
3	D	102	ILE
3	D	223	GLU
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	281/292 (96%)	265 (94%)	16 (6%)	18	20
1	B	284/292 (97%)	272 (96%)	12 (4%)	26	32
2	C	105/112 (94%)	102 (97%)	3 (3%)	37	47
2	E	106/112 (95%)	105 (99%)	1 (1%)	70	81
3	D	308/310 (99%)	297 (96%)	11 (4%)	31	39
3	F	312/310 (101%)	303 (97%)	9 (3%)	37	47
All	All	1396/1428 (98%)	1344 (96%)	52 (4%)	32	38

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP

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Mol	Chain	Res	Type
1	A	23	LEU
1	A	75	LEU
1	A	112[A]	VAL
1	A	112[B]	VAL
1	A	190	GLU
1	A	206	MET
1	A	232	GLU
1	A	256	GLU
1	A	300	ARG
1	A	303	GLU
1	A	306	ILE
1	A	321	ARG
1	A	357	LEU
1	A	358	LEU
1	A	359	GLU
1	B	60	GLN
1	B	102	GLN
1	B	157	GLU
1	B	167	GLU
1	B	219	THR
1	B	236	GLU
1	B	269	LEU
1	B	300[A]	ARG
1	B	300[B]	ARG
1	B	323	LEU
1	B	357	LEU
1	B	358	LEU
2	C	71	LEU
2	C	129	LYS
2	C	131	SER
3	D	92	ILE
3	D	106	GLU
3	D	117	VAL
3	D	127	LEU
3	D	208	THR
3	D	211	THR
3	D	218[A]	GLU
3	D	218[B]	GLU
3	D	262	LEU
3	D	265	VAL
3	D	354	LYS
2	E	71	LEU

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Mol	Chain	Res	Type
3	F	11[A]	GLN
3	F	11[B]	GLN
3	F	47	VAL
3	F	75	ILE
3	F	218	GLU
3	F	262	LEU
3	F	293	ARG
3	F	316	LEU
3	F	354	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	62	HIS
1	A	84	ASN
1	A	163	GLN
1	A	210	GLN
1	B	29	GLN
1	B	60	GLN
1	B	84	ASN
1	B	91	GLN
1	B	163	GLN
1	B	210	GLN
2	C	18	ASN
2	C	45	ASN
3	D	155	GLN
2	E	21	GLN
2	E	68	GLN
3	F	14	GLN
3	F	61	GLN
3	F	235	GLN
3	F	300	GLN
3	F	331	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	TRQ	E	57	2	16,17,18	2.09	4 (25%)	16,24,26	1.77	5 (31%)
2	TRQ	C	57	2	16,17,18	2.11	3 (18%)	16,24,26	1.66	6 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRQ	E	57	2	-	0/5/19/21	0/2/2/2
2	TRQ	C	57	2	-	0/5/19/21	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	57	TRQ	CE3-CD2	6.10	1.54	1.40
2	C	57	TRQ	CE3-CD2	5.59	1.53	1.40
2	C	57	TRQ	CE2-NE1	-3.83	1.32	1.38
2	E	57	TRQ	CE2-NE1	-3.17	1.33	1.38
2	C	57	TRQ	CB-CA	3.15	1.60	1.53
2	E	57	TRQ	CB-CA	2.98	1.59	1.53
2	E	57	TRQ	CZ3-CH2	-2.03	1.40	1.45

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	57	TRQ	CB-CG-CD1	-3.32	120.50	126.97
2	E	57	TRQ	CE2-CD2-CG	-3.15	102.99	107.16
2	E	57	TRQ	CD1-CG-CD2	2.79	108.47	105.95
2	C	57	TRQ	CE2-CD2-CG	-2.74	103.53	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	57	TRQ	CB-CG-CD1	-2.64	121.82	126.97
2	E	57	TRQ	O7-CZ2-CH2	2.44	121.50	118.39
2	E	57	TRQ	CD2-CE2-NE1	2.32	111.41	107.20
2	C	57	TRQ	CD2-CE2-NE1	2.29	111.37	107.20
2	C	57	TRQ	CD1-CG-CD2	2.29	108.02	105.95
2	C	57	TRQ	CE3-CZ3-CH2	-2.23	119.39	121.72
2	C	57	TRQ	CZ3-CH2-CZ2	2.12	121.73	118.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	57	TRQ	1	0
2	C	57	TRQ	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	1,10	46,50,50	2.60	22 (47%)	58,82,82	2.30	19 (32%)
7	EDO	B	406	-	3,3,3	0.62	0	2,2,2	0.21	0
7	EDO	B	405	-	3,3,3	0.27	0	2,2,2	0.34	0
9	MES	F	401	-	12,12,12	1.82	1 (8%)	15,16,16	2.45	5 (33%)
5	HEC	B	402	1,10	46,50,50	2.64	21 (45%)	58,82,82	2.67	19 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	HEC	A	403	1	46,50,50	2.56	19 (41%)	58,82,82	2.47	18 (31%)
8	ACT	D	401	-	3,3,3	0.93	0	3,3,3	1.51	0
5	HEC	B	403	1	46,50,50	2.38	19 (41%)	58,82,82	2.76	24 (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	1,10	-	4/14/54/54	-
7	EDO	B	406	-	-	1/1/1/1	-
7	EDO	B	405	-	-	1/1/1/1	-
9	MES	F	401	-	-	5/6/14/14	0/1/1/1
5	HEC	B	402	1,10	-	7/14/54/54	-
5	HEC	A	403	1	-	6/14/54/54	-
5	HEC	B	403	1	-	6/14/54/54	-

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	401	MES	C8-S	-5.76	1.69	1.77
5	A	403	HEC	CAC-C3C	5.66	1.53	1.35
5	B	402	HEC	CAB-C3B	5.29	1.52	1.35
5	A	402	HEC	CAC-C3C	5.17	1.51	1.35
5	B	402	HEC	CHD-C4C	5.16	1.48	1.38
5	A	402	HEC	CAB-C3B	5.08	1.51	1.35
5	A	402	HEC	CHC-C4B	5.06	1.48	1.38
5	B	403	HEC	CAB-C3B	4.99	1.51	1.35
5	B	402	HEC	CAC-C3C	4.98	1.51	1.35
5	B	402	HEC	CHA-C1A	4.97	1.48	1.38
5	A	403	HEC	CAB-C3B	4.94	1.51	1.35
5	B	403	HEC	CAC-C3C	4.81	1.50	1.35
5	A	402	HEC	CHA-C1A	4.67	1.47	1.38
5	B	402	HEC	CHB-C4A	4.58	1.47	1.38
5	A	402	HEC	CHD-C1D	4.53	1.49	1.39
5	A	403	HEC	C4A-NA	-4.49	1.31	1.39
5	B	403	HEC	CHA-C4D	4.47	1.49	1.39
5	A	403	HEC	CHB-C4A	4.45	1.47	1.38
5	B	403	HEC	CHD-C4C	4.44	1.47	1.38
5	A	402	HEC	CHD-C4C	4.40	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	403	HEC	CHC-C4B	4.32	1.46	1.38
5	B	403	HEC	CHB-C4A	4.29	1.46	1.38
5	A	402	HEC	CHB-C4A	4.29	1.46	1.38
5	A	403	HEC	CHA-C1A	4.19	1.46	1.38
5	A	403	HEC	CHC-C4B	4.18	1.46	1.38
5	A	403	HEC	CHA-C4D	4.10	1.48	1.39
5	B	403	HEC	C4D-ND	-4.05	1.32	1.39
5	A	403	HEC	CHD-C4C	4.04	1.46	1.38
5	A	402	HEC	CHA-C4D	4.01	1.48	1.39
5	B	402	HEC	C1D-ND	-3.90	1.32	1.39
5	B	402	HEC	C4B-NB	-3.84	1.32	1.39
5	A	402	HEC	CHB-C1B	3.82	1.48	1.39
5	A	402	HEC	CHC-C1C	3.82	1.48	1.39
5	B	402	HEC	CHD-C1D	3.74	1.47	1.39
5	A	403	HEC	C4B-NB	-3.67	1.32	1.39
5	B	402	HEC	C1C-NC	-3.64	1.32	1.39
5	A	403	HEC	C1B-NB	-3.63	1.32	1.39
5	B	402	HEC	C1B-NB	-3.63	1.32	1.39
5	B	402	HEC	CHA-C4D	3.52	1.47	1.39
5	A	403	HEC	C4C-NC	-3.51	1.33	1.39
5	B	403	HEC	CHC-C1C	3.49	1.47	1.39
5	B	402	HEC	CHB-C1B	3.45	1.47	1.39
5	B	403	HEC	CHA-C1A	3.43	1.45	1.38
5	B	402	HEC	CHC-C4B	3.39	1.45	1.38
5	A	403	HEC	CHC-C1C	3.37	1.47	1.39
5	A	402	HEC	C1D-ND	-3.28	1.33	1.39
5	B	402	HEC	C4A-NA	-3.27	1.33	1.39
5	A	403	HEC	CHD-C1D	3.26	1.46	1.39
5	A	403	HEC	C4D-ND	-3.24	1.33	1.39
5	A	402	HEC	C4C-NC	-3.18	1.33	1.39
5	B	402	HEC	CHC-C1C	3.16	1.46	1.39
5	A	402	HEC	C1A-NA	-3.10	1.33	1.39
5	B	402	HEC	C4C-NC	-3.06	1.33	1.39
5	A	402	HEC	C4D-ND	-2.95	1.34	1.39
5	B	403	HEC	C4B-NB	-2.90	1.34	1.39
5	B	402	HEC	C4D-ND	-2.89	1.34	1.39
5	A	403	HEC	C1A-NA	-2.84	1.34	1.39
5	A	403	HEC	C1C-NC	-2.84	1.34	1.39
5	B	403	HEC	C4C-NC	-2.82	1.34	1.39
5	B	403	HEC	CHD-C1D	2.79	1.45	1.39
5	B	402	HEC	C1B-C2B	2.71	1.49	1.43
5	A	403	HEC	CHB-C1B	2.70	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	403	HEC	C1D-ND	-2.68	1.34	1.39
5	A	402	HEC	C1B-C2B	2.67	1.49	1.43
5	A	402	HEC	C1B-NB	-2.65	1.34	1.39
5	A	402	HEC	C1D-C2D	2.61	1.49	1.43
5	B	403	HEC	C1D-ND	-2.50	1.34	1.39
5	B	403	HEC	C1B-NB	-2.45	1.35	1.39
5	A	402	HEC	C1A-C2A	2.40	1.49	1.45
5	B	403	HEC	O2D-CGD	-2.34	1.23	1.30
5	B	403	HEC	C1C-NC	-2.30	1.35	1.39
5	B	402	HEC	C4A-C3A	2.29	1.49	1.45
5	B	403	HEC	C1A-NA	-2.29	1.35	1.39
5	B	402	HEC	C1D-C2D	2.28	1.48	1.43
5	B	402	HEC	C3C-C4C	2.24	1.49	1.46
5	A	403	HEC	C1D-C2D	2.19	1.48	1.43
5	B	403	HEC	C1A-C2A	2.17	1.49	1.45
5	A	402	HEC	C1C-NC	-2.10	1.35	1.39
5	A	402	HEC	C4A-NA	-2.09	1.35	1.39
5	A	402	HEC	C4A-C3A	2.05	1.49	1.45
5	B	403	HEC	C4A-NA	-2.05	1.35	1.39
5	A	402	HEC	C3C-C4C	2.01	1.49	1.46

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	403	HEC	CBB-CAB-C3B	-11.96	103.52	127.43
5	B	402	HEC	CBB-CAB-C3B	-11.79	103.87	127.43
5	A	403	HEC	CBB-CAB-C3B	-10.22	107.00	127.43
5	B	403	HEC	CBC-CAC-C3C	-9.66	108.12	127.43
5	A	402	HEC	CBB-CAB-C3B	-8.74	109.96	127.43
5	A	403	HEC	CBC-CAC-C3C	-7.85	111.73	127.43
5	B	402	HEC	CBC-CAC-C3C	-7.55	112.35	127.43
5	A	402	HEC	CBC-CAC-C3C	-7.54	112.36	127.43
9	F	401	MES	C5-N4-C3	5.53	120.75	108.84
5	B	402	HEC	C3D-C4D-ND	5.15	115.86	110.15
5	A	403	HEC	CBD-CAD-C3D	-5.11	98.41	112.53
5	A	403	HEC	C2A-C1A-NA	4.47	114.63	110.32
5	B	403	HEC	C2A-C1A-NA	4.18	114.35	110.32
9	F	401	MES	C7-N4-C5	4.02	121.96	111.24
9	F	401	MES	O3S-S-C8	4.01	113.84	106.00
5	B	402	HEC	C2A-C1A-NA	3.98	114.17	110.32
5	B	402	HEC	CHC-C4B-NB	-3.96	120.15	124.45
5	A	402	HEC	C2A-C1A-NA	3.74	113.94	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	403	HEC	C3D-C4D-ND	3.62	114.17	110.15
9	F	401	MES	C2-C3-N4	-3.62	104.62	110.12
5	B	403	HEC	CBD-CAD-C3D	-3.62	102.54	112.53
5	A	402	HEC	C3D-C4D-ND	3.60	114.15	110.15
5	A	403	HEC	C1D-C2D-C3D	-3.58	102.71	106.82
5	B	402	HEC	C4D-C3D-C2D	-3.38	101.64	106.87
5	B	403	HEC	CMB-C2B-C3B	3.37	134.48	126.55
5	A	402	HEC	CHD-C4C-NC	-3.27	120.89	124.45
5	B	403	HEC	CMA-C3A-C4A	3.21	130.38	124.73
5	A	403	HEC	C1A-C2A-C3A	-3.15	102.96	107.11
5	B	402	HEC	CMB-C2B-C3B	3.04	133.71	126.55
5	B	403	HEC	C1D-C2D-C3D	-3.04	103.33	106.82
5	B	403	HEC	C2C-C1C-NC	3.01	114.97	110.14
5	B	403	HEC	C3A-C4A-NA	3.00	115.18	109.64
5	B	402	HEC	CMD-C2D-C3D	2.94	131.86	125.62
5	B	403	HEC	C2B-C1B-NB	2.87	114.74	110.14
5	B	403	HEC	CHB-C4A-NA	-2.85	121.34	124.45
5	B	402	HEC	CMC-C2C-C3C	2.84	133.23	126.55
5	B	402	HEC	O2A-CGA-CBA	2.80	122.85	114.00
5	A	403	HEC	C2D-C1D-ND	2.80	114.63	110.14
5	B	403	HEC	CBA-CAA-C2A	-2.80	104.79	112.53
5	A	402	HEC	CMA-C3A-C4A	2.77	129.60	124.73
5	B	402	HEC	C1A-C2A-C3A	-2.76	103.47	107.11
5	A	402	HEC	CHA-C1A-NA	-2.75	121.46	124.45
5	A	402	HEC	CHB-C4A-NA	-2.73	121.48	124.45
5	A	403	HEC	C3D-C4D-ND	2.69	113.14	110.15
5	A	403	HEC	CHB-C4A-NA	-2.69	121.52	124.45
5	A	403	HEC	C2B-C1B-NB	2.68	114.44	110.14
5	A	402	HEC	CBD-CAD-C3D	-2.68	105.12	112.53
5	B	402	HEC	C2B-C1B-NB	2.67	114.42	110.14
5	A	403	HEC	C2C-C1C-NC	2.66	114.41	110.14
5	A	403	HEC	O2A-CGA-CBA	2.63	122.31	114.00
5	A	402	HEC	C2C-C1C-NC	2.63	114.35	110.14
5	B	402	HEC	C2C-C1C-NC	2.63	114.35	110.14
5	A	403	HEC	CMB-C2B-C3B	2.62	132.72	126.55
5	A	402	HEC	C1D-C2D-C3D	-2.55	103.89	106.82
5	A	402	HEC	O2A-CGA-CBA	2.53	122.01	114.00
5	B	403	HEC	CAD-C3D-C4D	2.53	129.88	124.94
5	B	403	HEC	CHB-C1B-C2B	-2.52	120.10	127.43
5	A	403	HEC	CHD-C4C-NC	-2.47	121.76	124.45
5	A	402	HEC	C3A-C4A-NA	2.47	114.20	109.64
5	B	402	HEC	CHD-C4C-NC	-2.40	121.84	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	402	HEC	CMD-C2D-C1D	2.40	129.08	125.42
5	A	403	HEC	O1A-CGA-CBA	-2.36	115.61	123.09
5	A	402	HEC	CHC-C4B-NB	-2.34	121.90	124.45
5	A	402	HEC	C4A-C3A-C2A	-2.32	103.53	106.97
5	B	403	HEC	O2A-CGA-CBA	2.29	121.24	114.00
5	B	402	HEC	CAA-C2A-C1A	2.29	129.50	124.85
5	B	402	HEC	CHB-C4A-NA	-2.29	121.96	124.45
5	B	403	HEC	CHA-C1A-NA	-2.28	121.97	124.45
9	F	401	MES	C7-N4-C3	2.26	117.27	111.24
5	A	402	HEC	C2D-C1D-ND	2.26	113.76	110.14
5	B	403	HEC	C1A-C2A-C3A	-2.25	104.14	107.11
5	A	403	HEC	C3A-C4A-NA	2.20	113.71	109.64
5	A	402	HEC	CMC-C2C-C3C	2.20	131.71	126.55
5	B	402	HEC	CBD-CAD-C3D	-2.19	106.48	112.53
5	A	402	HEC	O1D-CGD-CBD	-2.18	116.18	123.09
5	B	402	HEC	C2D-C1D-ND	2.16	113.61	110.14
5	B	403	HEC	C2D-C1D-ND	2.16	113.60	110.14
5	B	403	HEC	C4A-C3A-C2A	-2.15	103.79	106.97
5	B	403	HEC	CHC-C1C-C2C	-2.14	121.22	127.43
5	A	403	HEC	CBA-CAA-C2A	-2.14	106.63	112.53
5	B	402	HEC	CHC-C1C-C2C	-2.13	121.26	127.43
5	B	403	HEC	C4A-NA-C1A	-2.02	102.53	105.82
5	B	403	HEC	CMD-C2D-C1D	2.01	128.48	125.42
5	A	403	HEC	CMD-C2D-C3D	2.01	129.89	125.62
5	B	403	HEC	CAD-CBD-CGD	-2.01	108.34	113.67

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	402	HEC	C2B-C3B-CAB-CBB
5	A	402	HEC	C4B-C3B-CAB-CBB
5	A	402	HEC	C2C-C3C-CAC-CBC
5	A	402	HEC	C4C-C3C-CAC-CBC
5	A	403	HEC	C2B-C3B-CAB-CBB
5	A	403	HEC	C4B-C3B-CAB-CBB
5	A	403	HEC	C2C-C3C-CAC-CBC
5	A	403	HEC	C4C-C3C-CAC-CBC
5	B	402	HEC	C2B-C3B-CAB-CBB
5	B	402	HEC	C4B-C3B-CAB-CBB
5	B	402	HEC	C2C-C3C-CAC-CBC
5	B	402	HEC	C4C-C3C-CAC-CBC

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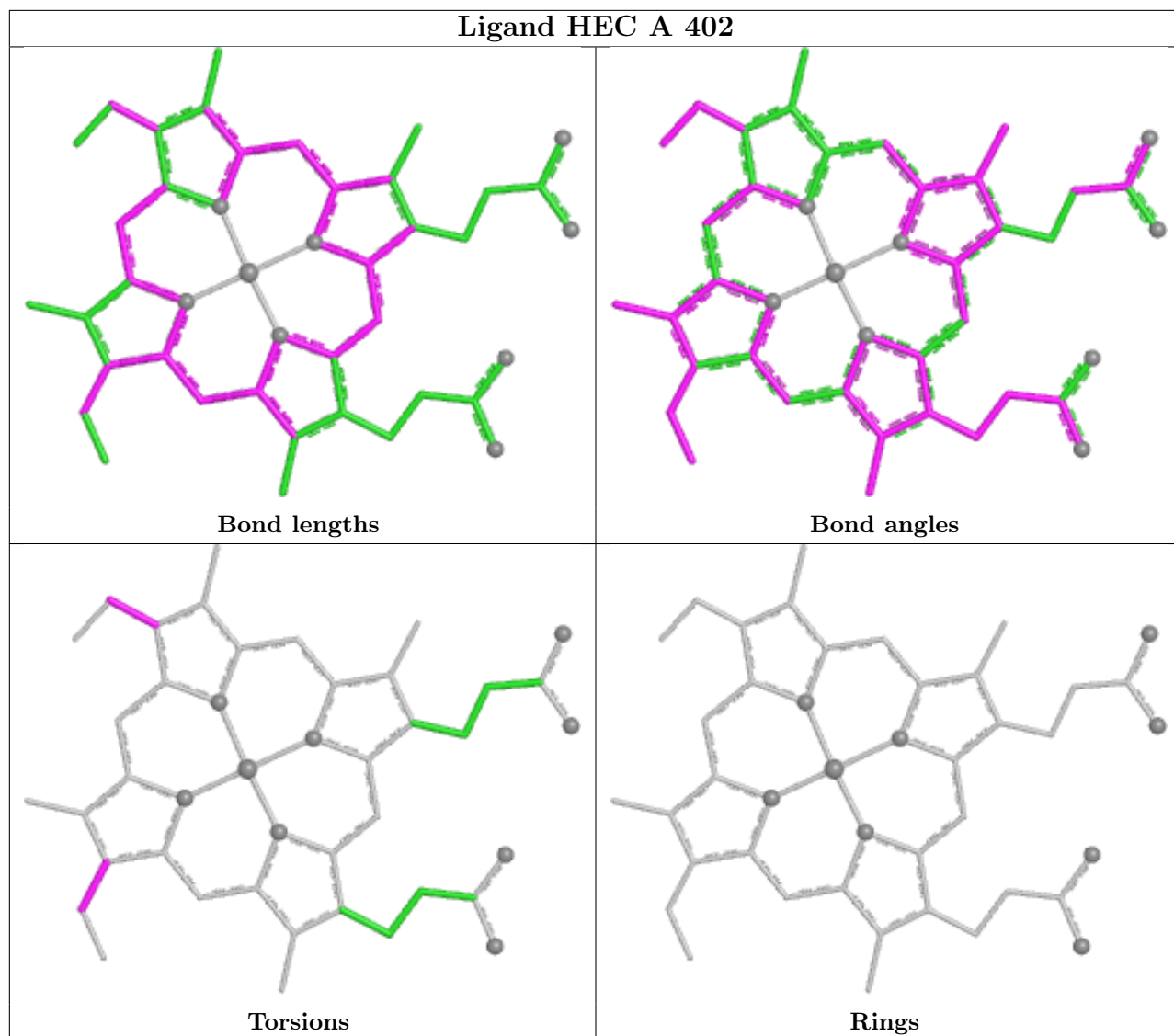
Mol	Chain	Res	Type	Atoms
5	B	403	HEC	C2B-C3B-CAB-CBB
5	B	403	HEC	C4B-C3B-CAB-CBB
5	B	403	HEC	C2C-C3C-CAC-CBC
5	B	403	HEC	C4C-C3C-CAC-CBC
9	F	401	MES	C8-C7-N4-C5
9	F	401	MES	N4-C7-C8-S
9	F	401	MES	C7-C8-S-O1S
9	F	401	MES	C7-C8-S-O3S
7	B	405	EDO	O1-C1-C2-O2
9	F	401	MES	C7-C8-S-O2S
5	A	403	HEC	CAD-CBD-CGD-O2D
5	B	402	HEC	CAA-CBA-CGA-O2A
5	B	402	HEC	CAA-CBA-CGA-O1A
5	B	402	HEC	C3D-CAD-CBD-CGD
5	A	403	HEC	CAD-CBD-CGD-O1D
5	B	403	HEC	CAD-CBD-CGD-O2D
5	B	403	HEC	CAD-CBD-CGD-O1D
7	B	406	EDO	O1-C1-C2-O2

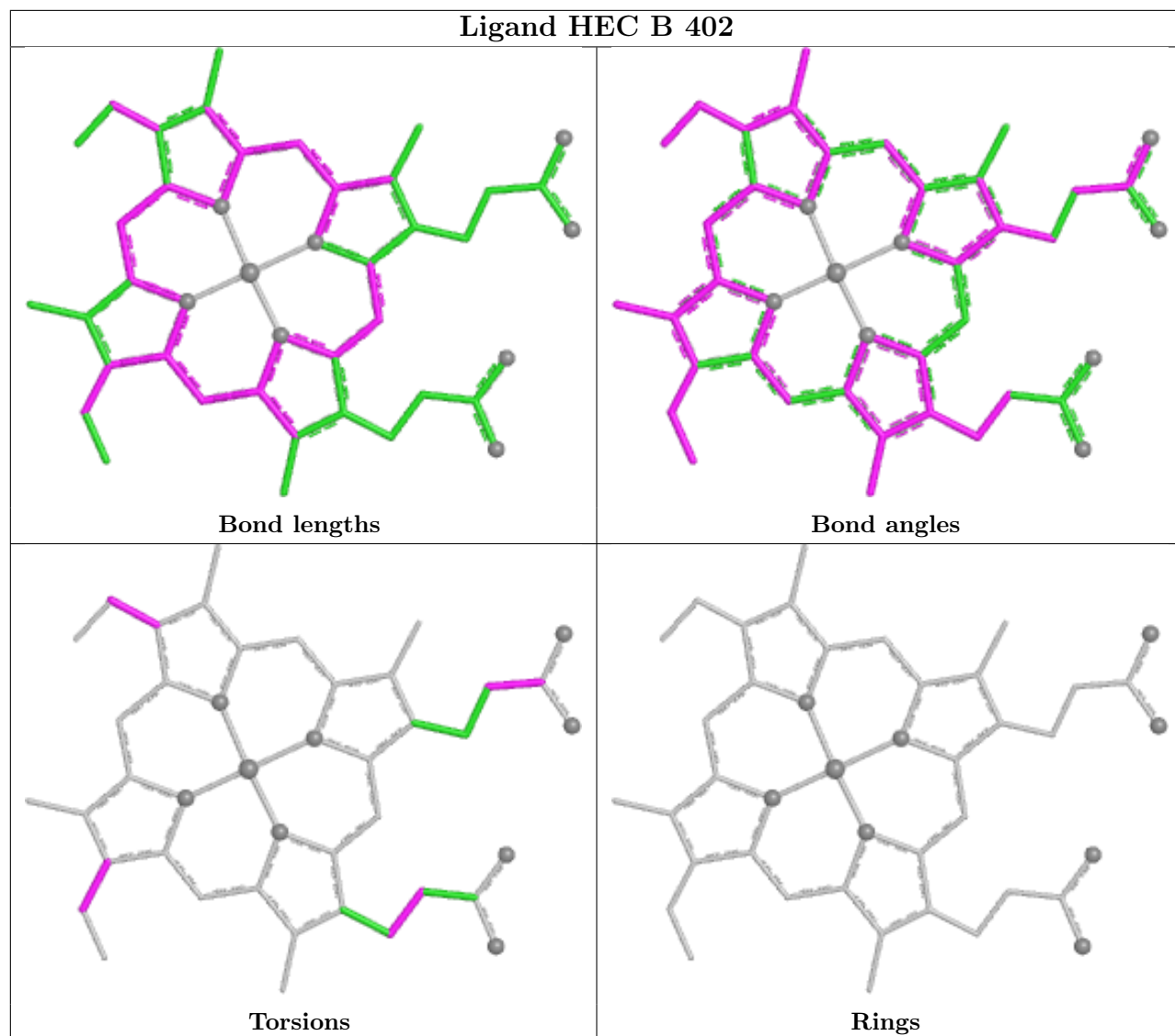
There are no ring outliers.

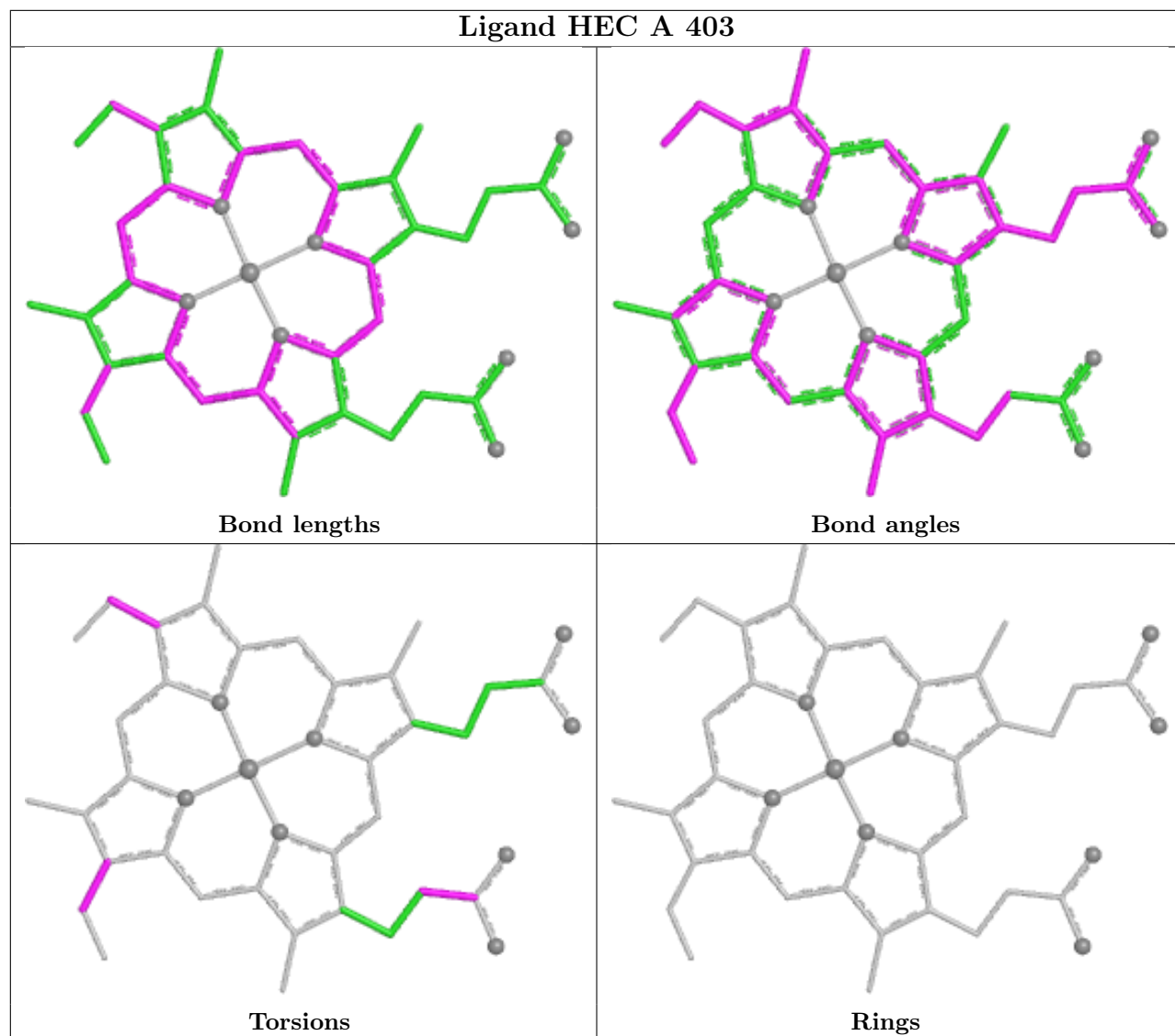
5 monomers are involved in 11 short contacts:

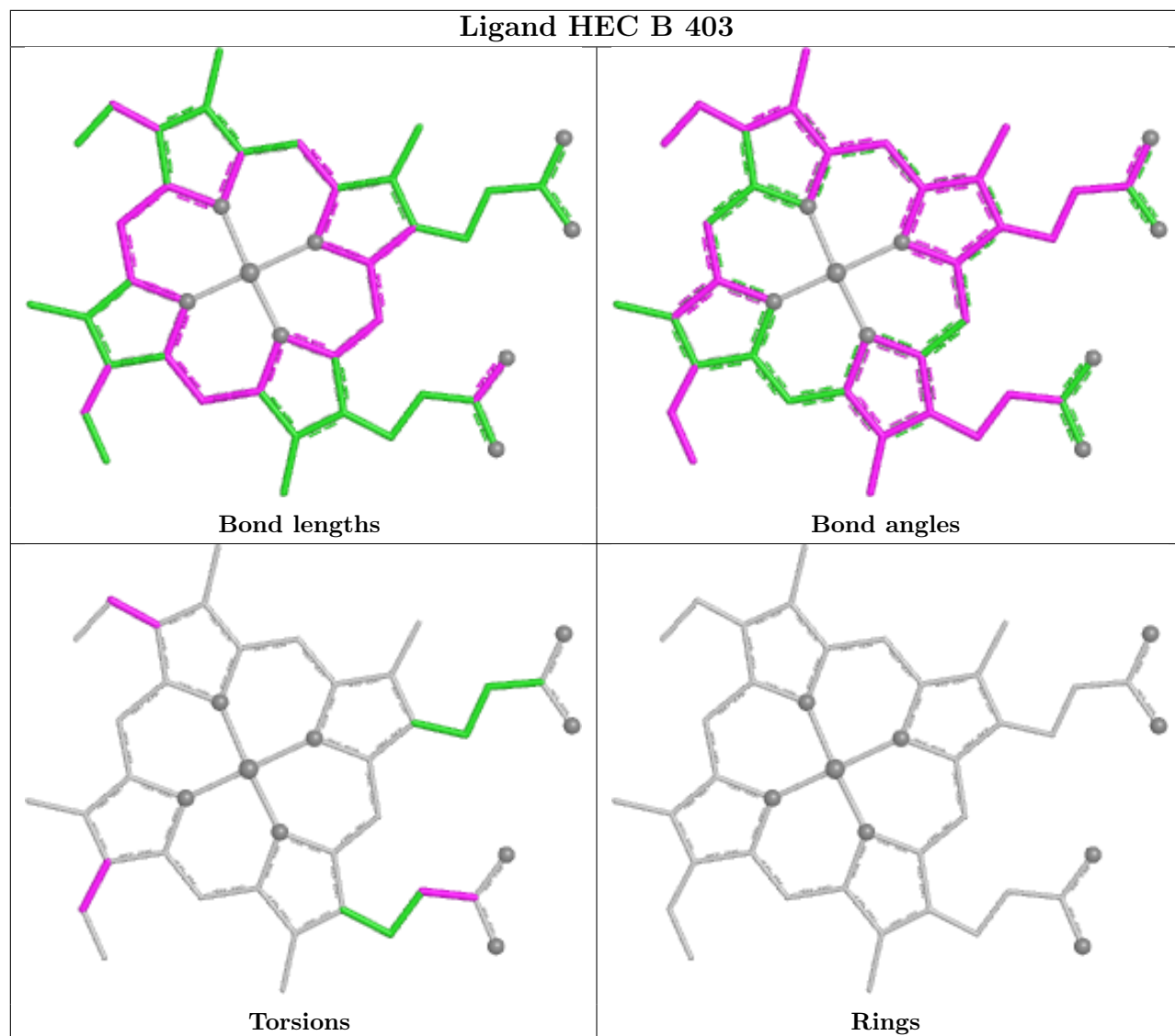
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	402	HEC	4	0
7	B	405	EDO	2	0
5	B	402	HEC	2	0
5	A	403	HEC	1	0
5	B	403	HEC	2	0

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 [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	354/373 (94%)	-0.19	1 (0%) 90 89	18, 42, 61, 72	5 (1%)
1	B	355/373 (95%)	-0.44	1 (0%) 90 89	14, 35, 53, 75	7 (1%)
2	C	124/137 (90%)	-0.31	1 (0%) 82 82	22, 36, 57, 74	1 (0%)
2	E	124/137 (90%)	-0.59	1 (0%) 82 82	14, 27, 39, 65	2 (1%)
3	D	376/385 (97%)	-0.17	0 100 100	24, 43, 71, 83	4 (1%)
3	F	376/385 (97%)	-0.60	2 (0%) 87 86	13, 29, 47, 61	8 (2%)
All	All	1709/1790 (95%)	-0.37	6 (0%) 88 88	13, 36, 61, 83	27 (1%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	11[A]	GLN	3.4
1	A	6	ALA	3.0
2	C	131	SER	2.6
1	B	84	ASN	2.5
3	F	207	GLY	2.2
2	E	131	SER	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	C	57	16/17	0.92	0.10	41,48,53,58	0
2	TRQ	E	57	16/17	0.93	0.09	33,38,45,47	0

6.3 Carbohydrates [i](#)

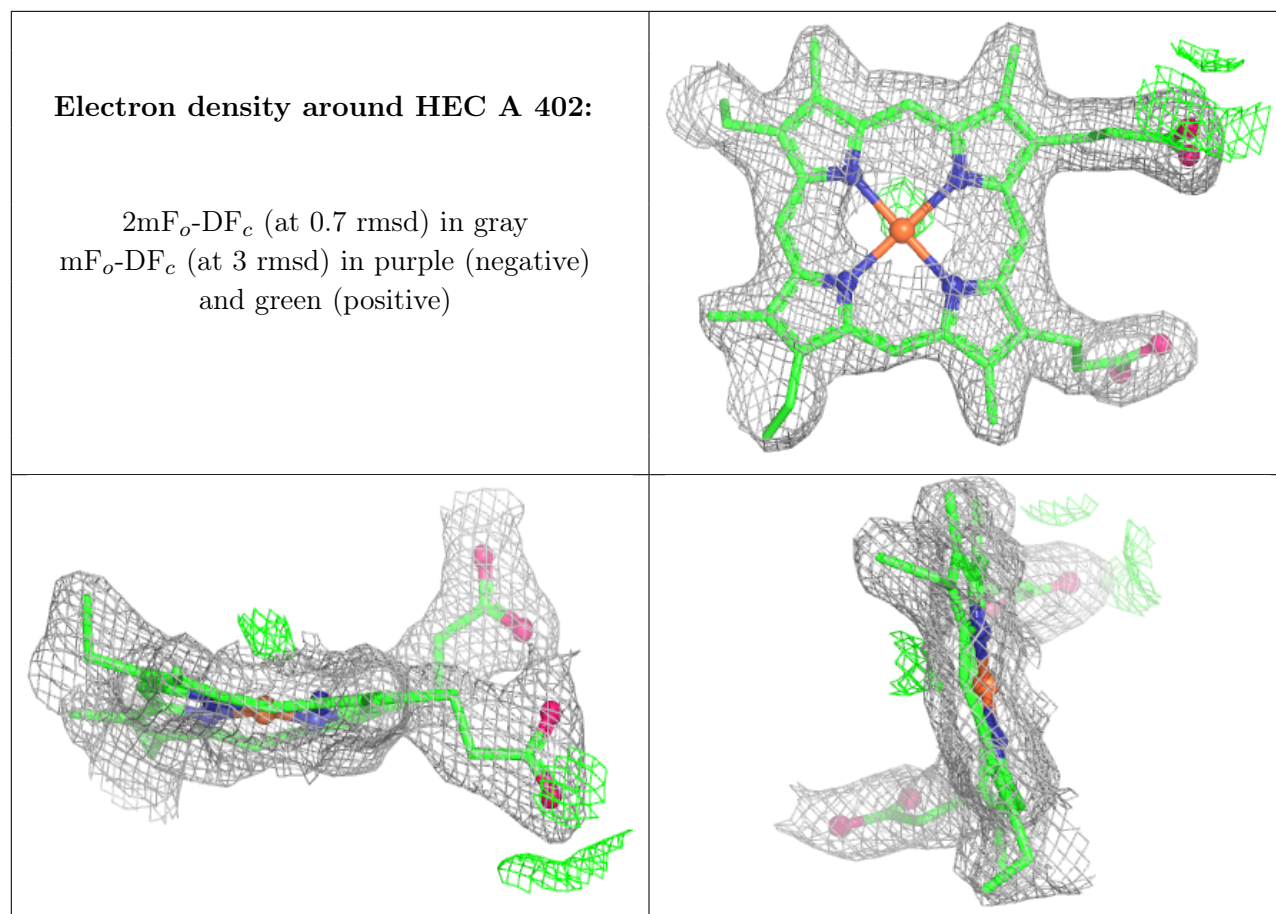
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

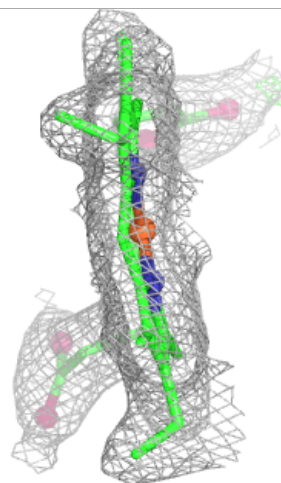
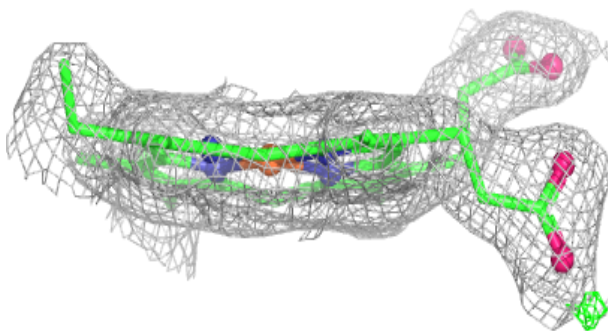
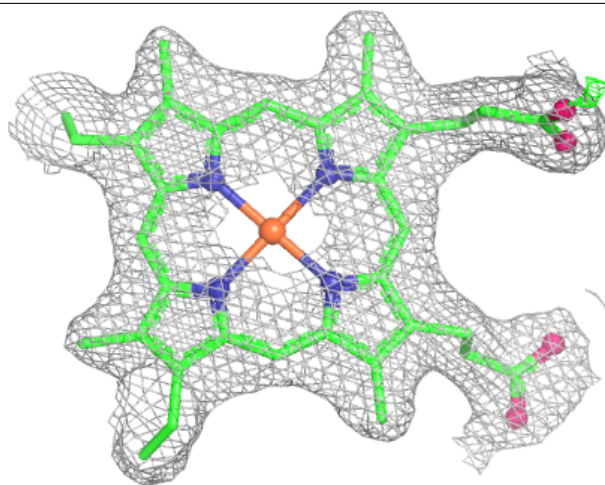
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NA	A	404	1/1	0.80	0.19	58,58,58,58	0
7	EDO	B	406	4/4	0.81	0.18	59,60,60,60	0
9	MES	F	401	12/12	0.85	0.14	73,78,79,79	0
8	ACT	D	401	4/4	0.89	0.12	48,50,51,51	0
6	NA	B	404	1/1	0.93	0.04	42,42,42,42	0
7	EDO	B	405	4/4	0.94	0.10	44,45,46,48	0
5	HEC	A	402	43/43	0.98	0.07	27,36,38,39	0
5	HEC	A	403	43/43	0.98	0.06	30,34,39,43	0
5	HEC	B	402	43/43	0.98	0.06	22,29,33,34	0
4	CA	B	401	1/1	0.99	0.02	26,26,26,26	0
4	CA	A	401	1/1	0.99	0.02	40,40,40,40	0
5	HEC	B	403	43/43	0.99	0.05	15,21,26,31	0

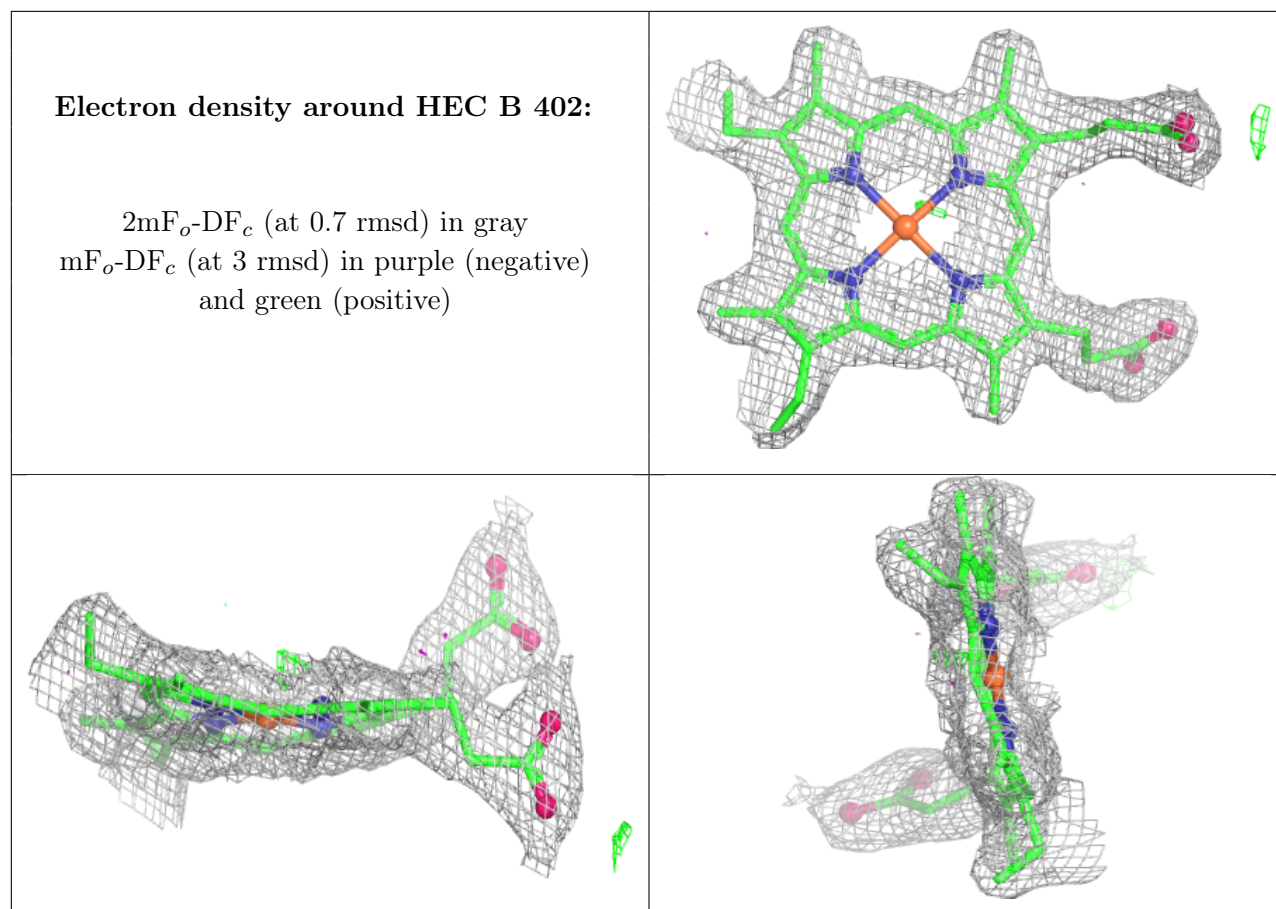
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

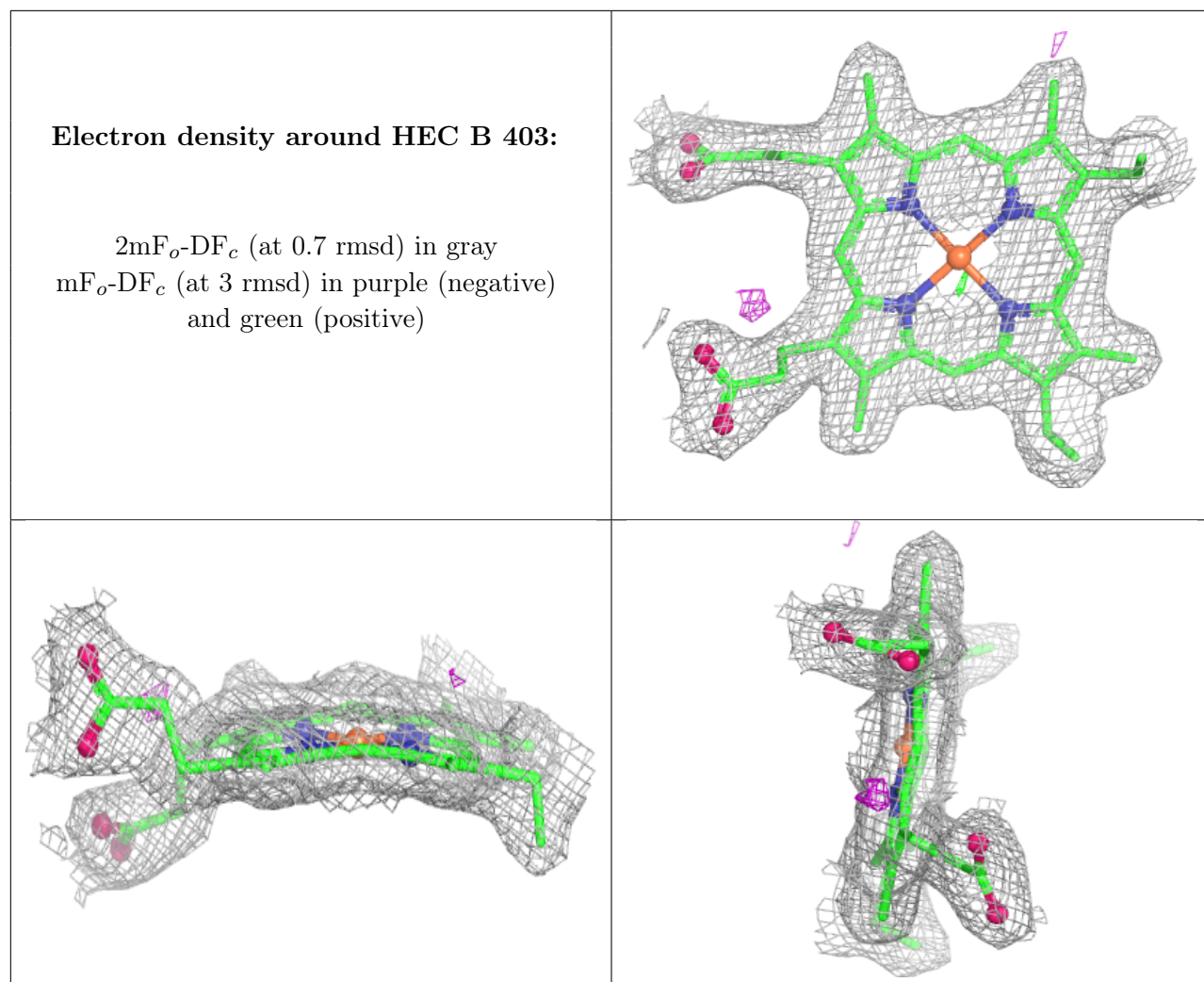


Electron density around HEC A 403:

$2mF_o-DF_c$ (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.