



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:46 AM UTC

PDB ID : 4FA9 / pdb_00004fa9
Title : Crystal Structure of WT MauG in Complex with Pre-Methylamine Dehydrogenase Aged 30 Days
Authors : Yukl, E.T.; Wilmot, C.M.
Deposited on : 2012-05-21
Resolution : 2.09 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)
Xtrriage (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

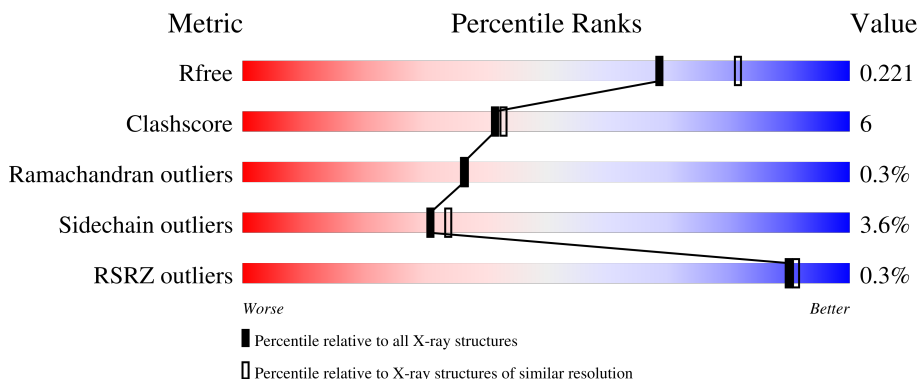
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	 78% 14% • 5%
1	B	373	 87% 9% • •
2	C	137	 78% 13% •• 6%
2	E	137	 70% 20% • 8%
3	D	385	 76% 19% ••

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Mol	Chain	Length	Quality of chain
3	F	385	 85% 11% ..

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14575 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	3	0
			2760	1722	496	531	11			
1	B	357	Total	C	N	O	S	0	3	0
			2788	1736	503	538	11			

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	129	Total	C	N	O	S	0	4	0
			1034	644	178	198	14			
2	E	126	Total	C	N	O	S	0	4	0
			999	621	167	197	14			

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
			Total	C	N	O	S			
3	D	376	Total	C	N	O	S	0	3	0
			2954	1870	511	565	8			
3	F	376	Total	C	N	O	S	0	4	0
			2955	1871	509	566	9			

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

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

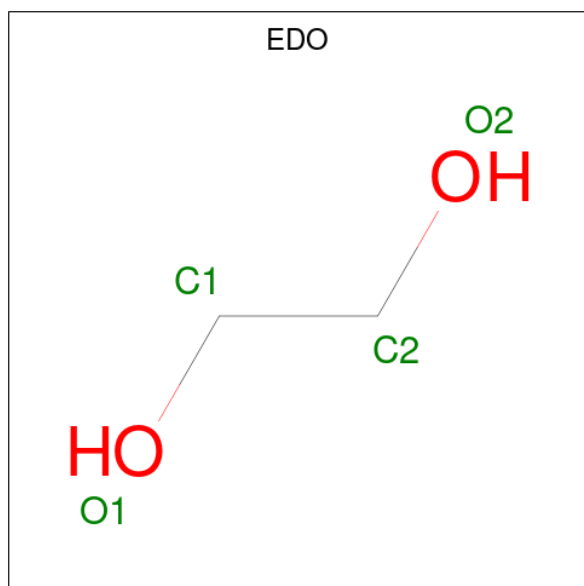
- Molecule 5 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	F	1	Total C O 4 2 2	0	0

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

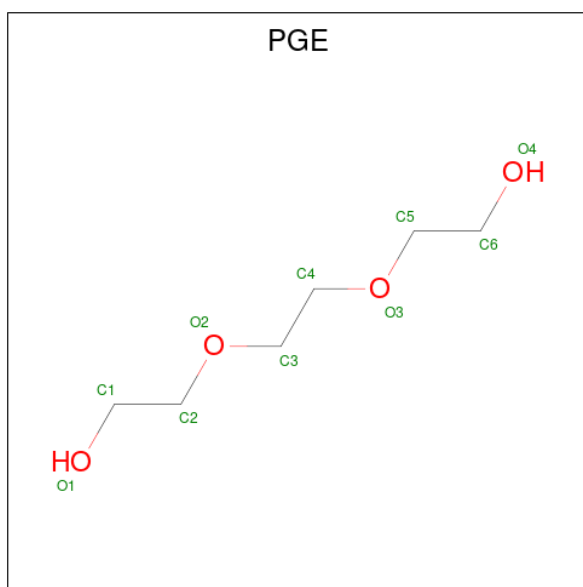
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Na 2 2	0	0
7	B	2	Total Na 2 2	0	0

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 9 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).




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

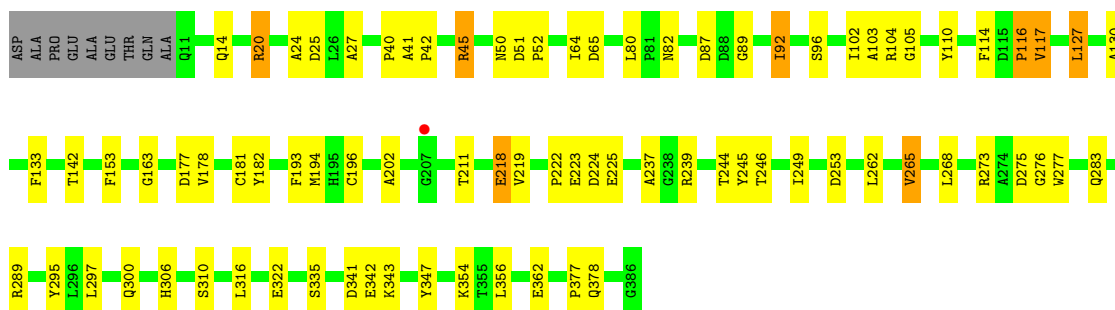
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	127	Total	O	0	1
			128	128		
10	B	203	Total	O	0	1
			204	204		
10	C	53	Total	O	0	0
			53	53		
10	D	160	Total	O	0	0
			160	160		
10	E	74	Total	O	0	0
			74	74		
10	F	254	Total	O	0	0
			254	254		


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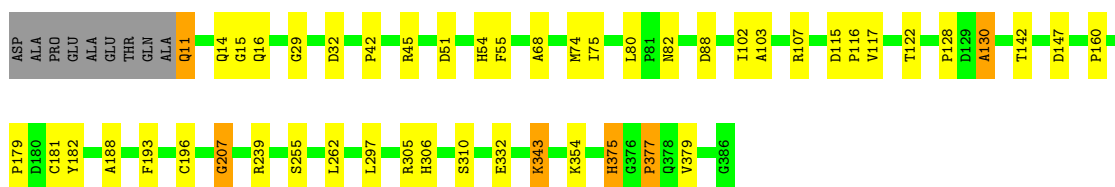
• Molecule 3: Methylamine dehydrogenase heavy chain

Chain D:  76% 19% ..



• Molecule 3: Methylamine dehydrogenase heavy chain

Chain F:  85% 11% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.53Å 83.54Å 107.78Å 109.94° 91.54° 105.78°	Depositor
Resolution (Å)	44.49 – 2.09 44.49 – 2.09	Depositor EDS
% Data completeness (in resolution range)	97.6 (44.49-2.09) 97.6 (44.49-2.09)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.08Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.157 , 0.214 0.166 , 0.221	Depositor DCC
R_{free} test set	5175 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	34.8	Xtrriage
Anisotropy	0.049	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.3	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	0.97	EDS
Total number of atoms	14575	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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: PGE, CA, EDO, ACT, 0AF, HEC, 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	1.16	4/2827 (0.1%)	1.18	12/3835 (0.3%)
1	B	1.27	2/2852 (0.1%)	1.15	4/3868 (0.1%)
2	C	1.15	0/1037	1.14	0/1417
2	E	1.34	3/998 (0.3%)	1.24	0/1363
3	D	1.17	6/3031 (0.2%)	1.10	9/4128 (0.2%)
3	F	1.38	16/3035 (0.5%)	1.19	3/4134 (0.1%)
All	All	1.25	31/13780 (0.2%)	1.16	28/18745 (0.1%)

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	80	LEU	C-O	-8.28	1.19	1.23
3	F	130	ALA	N-CA	8.20	1.52	1.46
3	F	103	ALA	CA-CB	7.07	1.64	1.53
3	F	377	PRO	CA-C	6.95	1.61	1.52
3	D	103	ALA	CA-CB	6.47	1.64	1.54
3	D	27	ALA	CA-CB	6.32	1.63	1.53
2	E	60	SER	N-CA	-6.22	1.38	1.46
3	D	130	ALA	N-CA	5.92	1.50	1.46
2	E	86	CYS	C-O	-5.88	1.21	1.23
3	F	379	VAL	C-O	5.88	1.30	1.24
2	E	124	SER	CA-CB	5.72	1.59	1.53
3	F	115	ASP	CA-C	5.71	1.59	1.52
3	F	68	ALA	CA-CB	5.61	1.63	1.53
3	D	64	ILE	C-O	5.59	1.29	1.24
1	A	164	ALA	CA-CB	5.59	1.63	1.53
3	F	193	PHE	CA-C	-5.54	1.46	1.52
1	A	104	ALA	CA-CB	5.51	1.62	1.53
3	F	207	GLY	C-O	5.50	1.29	1.23
3	F	80	LEU	N-CA	5.46	1.50	1.46
1	A	122	VAL	CA-CB	5.43	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	24	ALA	CA-CB	5.40	1.62	1.53
3	F	188	ALA	CA-CB	5.32	1.61	1.54
3	F	122	THR	CA-CB	-5.29	1.46	1.54
3	F	377	PRO	N-CA	-5.26	1.40	1.47
3	F	117	VAL	C-O	-5.26	1.18	1.23
1	B	339	VAL	CA-CB	5.25	1.61	1.54
3	D	87	ASP	CA-C	-5.12	1.45	1.52
3	F	239	ARG	CA-C	-5.09	1.46	1.52
1	A	112	VAL	CA-CB	5.07	1.60	1.54
3	F	128	PRO	C-O	5.06	1.29	1.23
1	B	127	ARG	C-O	-5.02	1.17	1.24

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	ASN	N-CA-C	9.42	122.73	111.33
1	A	7	ASP	N-CA-C	-8.79	101.82	112.54
1	A	169	SER	CA-C-N	-8.19	111.19	120.04
1	A	169	SER	C-N-CA	-8.19	111.19	120.04
3	D	127	LEU	CA-C-N	-7.13	112.65	119.85
3	D	127	LEU	C-N-CA	-7.13	112.65	119.85
3	D	244	THR	N-CA-C	-6.72	100.28	109.95
1	B	186	THR	CA-C-N	-5.87	112.83	119.28
1	B	186	THR	C-N-CA	-5.87	112.83	119.28
1	A	336	ASP	CA-C-N	5.83	126.57	119.99
1	A	336	ASP	C-N-CA	5.83	126.57	119.99
3	D	25	ASP	N-CA-C	-5.71	104.97	111.14
3	F	332	GLU	CA-C-N	-5.56	116.30	123.19
3	F	332	GLU	C-N-CA	-5.56	116.30	123.19
1	A	167	GLU	N-CA-C	5.53	117.31	111.28
3	D	116	PRO	CA-C-N	-5.47	117.35	122.66
3	D	116	PRO	C-N-CA	-5.47	117.35	122.66
1	A	197	ILE	N-CA-C	5.41	119.02	112.80
1	B	294	TYR	N-CA-C	5.41	117.92	111.71
3	D	65	ASP	N-CA-C	-5.36	99.79	108.41
1	B	15	ALA	N-CA-C	-5.31	105.49	111.28
1	A	174	LYS	N-CA-C	-5.28	105.53	111.28
3	D	245	TYR	N-CA-C	5.27	118.81	112.38
1	A	43	ASP	CA-C-N	5.10	124.71	119.56
1	A	43	ASP	C-N-CA	5.10	124.71	119.56
3	F	375	HIS	N-CA-C	-5.08	107.63	113.88
1	A	121	ALA	N-CA-C	-5.08	105.83	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	80	LEU	CB-CA-C	-5.05	107.61	111.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2760	0	2632	38	0
1	B	2788	0	2653	14	0
2	C	1034	0	917	36	0
2	E	999	0	887	27	0
3	D	2954	0	2837	44	0
3	F	2955	0	2837	32	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	86	0	60	1	0
5	B	86	0	60	1	0
6	A	8	0	6	0	0
6	B	4	0	3	0	0
6	D	4	0	3	0	0
6	F	4	0	3	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
8	B	4	0	6	0	0
9	F	10	0	14	1	0
10	A	128	0	0	2	0
10	B	204	0	0	0	0
10	C	53	0	0	2	0
10	D	160	0	0	5	0
10	E	74	0	0	3	0
10	F	254	0	0	3	0
All	All	14575	0	12918	170	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 6.

All (170) 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)
2:C:130:ALA:HA	2:C:131:SER:HB2	1.22	1.20
2:C:130:ALA:CA	2:C:131:SER:HB2	1.70	1.16
2:E:6:GLY:O	2:E:7:THR:HG23	1.46	1.13
2:E:6:GLY:O	2:E:7:THR:CG2	2.03	1.05
2:C:130:ALA:CB	2:C:131:SER:HB2	1.91	1.00
2:C:131:SER:HB3	10:C:243:HOH:O	1.67	0.94
2:C:130:ALA:HB1	2:C:131:SER:CB	1.99	0.92
1:B:82:ASP:OD1	1:B:84:ASN:HB2	1.68	0.91
2:C:57[B]:0AF:HBC1	2:C:108[B]:TRP:NE1	1.88	0.88
1:B:285:THR:HG22	1:B:286:ASP:OD1	1.77	0.84
1:A:197:ILE:O	1:A:202[B]:ARG:HD2	1.78	0.84
2:E:6:GLY:C	2:E:7:THR:CG2	2.50	0.84
2:E:6:GLY:C	2:E:7:THR:HG22	2.06	0.80
2:E:57[B]:0AF:HBC1	2:E:108[B]:TRP:NE1	1.96	0.79
2:C:130:ALA:CB	2:C:131:SER:CB	2.60	0.79
3:D:342:GLU:HA	10:D:612:HOH:O	1.81	0.79
1:A:210:GLN:HE22	2:C:44:THR:HG21	1.49	0.78
2:E:57[A]:0AF:CE3	2:E:108[A]:TRP:CD1	2.67	0.78
2:C:130:ALA:HB1	2:C:131:SER:HB3	1.64	0.78
3:F:11:GLN:HA	3:F:11:GLN:OE1	1.83	0.77
3:F:207:GLY:HA3	10:F:745:HOH:O	1.85	0.77
2:C:57[A]:0AF:CE3	2:C:108[A]:TRP:CD1	2.69	0.76
3:F:181[B]:CYS:HB3	3:F:196:CYS:SG	2.26	0.74
2:C:130:ALA:HA	2:C:131:SER:CB	2.13	0.72
1:A:48:LYS:H	1:A:62:HIS:HE1	1.36	0.72
2:C:129:LYS:O	2:C:130:ALA:HB3	1.90	0.69
2:E:57[B]:0AF:HBC1	2:E:108[B]:TRP:HE1	1.57	0.69
2:E:6:GLY:O	2:E:7:THR:HG22	1.93	0.68
1:A:197:ILE:CD1	2:C:71:LEU:HD23	2.25	0.67
2:C:129:LYS:O	2:C:130:ALA:CB	2.44	0.66
1:A:301:ARG:CZ	1:A:333:MET:HE1	2.26	0.66
1:A:206:MET:HA	1:A:206:MET:HE2	1.77	0.66
2:E:101[A]:GLU:HA	10:E:260:HOH:O	1.96	0.65
3:D:362:GLU:HA	3:D:362:GLU:OE1	1.97	0.64
2:E:131:SER:HA	10:E:235:HOH:O	1.98	0.64
2:C:57[A]:0AF:HE3	2:C:108[A]:TRP:CD1	2.33	0.64
2:E:11:ALA:O	3:F:305[B]:ARG:HD2	1.99	0.64
1:B:210:GLN:HE22	2:E:44:THR:HG21	1.62	0.63
3:F:343:LYS:N	3:F:343:LYS:HD3	2.13	0.62
1:A:48:LYS:H	1:A:62:HIS:CE1	2.19	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:42:PRO:HD3	3:D:117:VAL:HG12	1.83	0.60
2:C:57[B]:0AF:HBC1	2:C:108[B]:TRP:HE1	1.63	0.59
3:F:51:ASP:HA	3:F:377:PRO:HA	1.85	0.59
1:A:208:ARG:NH2	3:F:29:GLY:O	2.37	0.58
3:D:45:ARG:NH2	3:D:343:LYS:O	2.37	0.57
1:A:110:ASN:OD1	1:A:112:VAL:HG13	2.04	0.57
1:B:299:SER:HB3	1:B:304:ALA:CB	2.34	0.57
1:A:301:ARG:NH1	1:A:333:MET:HE1	2.19	0.57
3:D:275:ASP:HB2	10:D:625:HOH:O	2.06	0.56
1:A:197:ILE:HD12	2:C:71:LEU:HD23	1.88	0.56
1:A:21:PRO:O	1:A:27:ALA:HA	2.06	0.56
1:A:60:GLN:O	1:A:62:HIS:HD2	1.88	0.56
3:D:347:TYR:HB3	3:D:356:LEU:HD11	1.88	0.55
3:D:341:ASP:OD1	3:D:341:ASP:N	2.31	0.54
2:E:57[A]:0AF:HE3	2:E:108[A]:TRP:CD1	2.43	0.54
3:D:51:ASP:HA	3:D:377:PRO:HA	1.89	0.54
2:C:61:CYS:HB2	2:C:72[B]:ILE:HD12	1.90	0.54
3:D:237:ALA:HB2	3:D:289:ARG:HG3	1.90	0.54
3:F:297:LEU:HD22	3:F:310:SER:HB2	1.90	0.53
3:D:20[A]:ARG:NH1	10:D:633:HOH:O	2.42	0.53
3:F:82:ASN:HB3	3:F:142:THR:HB	1.90	0.53
3:D:42:PRO:HG3	3:D:116:PRO:HB2	1.91	0.52
2:C:21:GLN:HE22	3:F:14[A]:GLN:HE21	1.58	0.52
3:D:268:LEU:HD22	3:D:277:TRP:HB3	1.92	0.52
2:E:56:SER:CB	2:E:74:TYR:O	2.58	0.51
3:D:52:PRO:HG2	3:D:378:GLN:OE1	2.11	0.51
3:D:92:ILE:HG12	3:D:114:PHE:HB2	1.93	0.50
3:F:343:LYS:HD3	3:F:343:LYS:H	1.76	0.50
3:D:239[B]:ARG:HH11	3:D:239[B]:ARG:HA	1.77	0.50
1:A:110:ASN:OD1	1:A:112:VAL:CG1	2.60	0.50
2:C:106:ILE:HG12	3:D:133:PHE:CZ	2.47	0.50
2:C:91:THR:HB	3:D:306:HIS:CE1	2.46	0.50
3:D:14:GLN:HE21	2:E:21:GLN:HE22	1.59	0.50
1:B:355:GLU:O	1:B:358:LEU:HB2	2.12	0.49
1:A:210:GLN:NE2	2:C:44:THR:HG21	2.24	0.49
1:B:91:GLN:O	1:B:92:PHE:HB2	2.11	0.49
3:D:20[A]:ARG:HA	3:D:20[A]:ARG:NE	2.28	0.49
3:F:45:ARG:NH2	3:F:343:LYS:O	2.45	0.49
2:C:75:ARG:HA	10:C:247:HOH:O	2.12	0.49
1:A:223:TYR:CE2	1:A:265:LYS:HB2	2.47	0.49
3:D:193:PHE:HA	3:D:202:ALA:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:50:ASN:HB3	10:D:605:HOH:O	2.11	0.49
2:C:21:GLN:HE22	3:F:14[A]:GLN:NE2	2.10	0.48
1:A:197:ILE:HD11	2:C:71:LEU:HD23	1.95	0.48
1:A:208:ARG:HH22	3:F:29:GLY:C	2.22	0.48
1:A:353:ARG:HH11	1:A:353:ARG:HG2	1.79	0.48
1:B:288:ARG:NH1	1:B:340:ASP:OD1	2.44	0.48
2:E:19:ASP:O	2:E:25:TYR:HB2	2.14	0.47
3:F:147:ASP:OD1	3:F:147:ASP:C	2.57	0.47
1:A:40:ALA:HA	1:A:354:TYR:CZ	2.49	0.47
2:E:23:CYS:SG	2:E:88[B]:CYS:HB2	2.54	0.47
2:E:101[B]:GLU:HG2	2:E:102:PHE:CD2	2.49	0.47
3:F:42:PRO:HG3	3:F:116:PRO:HB2	1.97	0.47
3:D:297:LEU:HD22	3:D:310:SER:HB2	1.95	0.47
3:F:305[B]:ARG:NH1	10:F:727:HOH:O	2.42	0.47
2:C:57[B]:OAF:HBC1	2:C:108[B]:TRP:CE2	2.49	0.47
3:D:277:TRP:CE2	3:D:300:GLN:HG3	2.49	0.47
3:F:107:ARG:HD3	3:F:130:ALA:HB1	1.96	0.47
1:B:113:GLU:HG2	5:B:402:HEC:HBC2	1.96	0.47
3:D:222:PRO:HG2	3:D:225:GLU:HB2	1.95	0.47
1:A:71:GLY:HA2	1:A:168:PHE:O	2.15	0.47
1:A:303[B]:GLU:CD	1:A:303[B]:GLU:H	2.22	0.47
1:B:52:ALA:O	1:B:66:ASN:HA	2.15	0.47
3:D:181:CYS:C	3:D:182:TYR:CD1	2.93	0.47
3:D:239[B]:ARG:NH1	3:D:253:ASP:OD1	2.48	0.47
1:A:277:PRO:HB3	1:A:285:THR:HA	1.96	0.46
3:D:96:SER:HB3	3:D:110:TYR:CZ	2.50	0.46
2:E:33:GLY:HA3	2:E:119:TYR:OH	2.15	0.46
2:E:96:PRO:HB2	2:E:98:TYR:CE1	2.51	0.46
1:A:91:GLN:O	1:A:92:PHE:HB2	2.15	0.46
3:F:54:HIS:HE1	10:F:717:HOH:O	1.98	0.46
1:B:299:SER:HB2	1:B:333:MET:HG3	1.98	0.46
3:D:249:ILE:HB	3:D:265:VAL:HG12	1.98	0.45
2:E:71:LEU:CD2	2:E:129:LYS:O	2.64	0.45
1:A:172:ASP:O	1:A:177:ARG:NH1	2.50	0.45
1:A:281:ASN:OD1	1:A:283:VAL:HG12	2.17	0.45
2:C:106:ILE:HG12	3:D:133:PHE:HZ	1.81	0.45
3:D:283:GLN:HB2	3:D:335:SER:HB3	1.99	0.44
1:A:65:ARG:HH12	1:A:94:ASP:CG	2.25	0.44
3:D:283:GLN:HB2	3:D:335:SER:CB	2.48	0.44
1:B:278:TYR:O	1:B:279:MET:HB2	2.16	0.44
3:D:246:THR:O	3:D:273:ARG:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:305[A]:ARG:HA	3:F:305[A]:ARG:HD2	1.76	0.44
1:A:19:VAL:HG13	10:A:530:HOH:O	2.16	0.44
2:C:19:ASP:OD1	3:F:15:GLY:HA3	2.16	0.44
2:C:78:CYS:HA	2:C:118:THR:O	2.18	0.44
3:F:255:SER:HA	9:F:402:PGE:H62	1.98	0.44
3:D:253:ASP:HB2	3:D:262:LEU:CD1	2.48	0.44
1:A:197:ILE:HA	1:A:202[A]:ARG:HB3	2.00	0.43
3:D:82:ASN:HB3	3:D:142:THR:HB	2.00	0.43
2:C:57[B]:OAF:CB	2:C:108[B]:TRP:NE1	2.73	0.43
3:D:239[B]:ARG:HH11	3:D:239[B]:ARG:CA	2.32	0.43
3:F:179:PRO:HD2	3:F:181[B]:CYS:SG	2.57	0.43
1:A:175:TYR:CD2	1:A:175:TYR:C	2.96	0.43
3:D:40:PRO:O	3:D:41:ALA:C	2.60	0.43
2:E:31:ILE:HD13	2:E:31:ILE:HG21	1.68	0.43
1:A:223:TYR:CG	1:A:249:LEU:HD22	2.53	0.43
2:E:9:PRO:O	3:F:305[B]:ARG:HD3	2.18	0.43
2:C:58:VAL:HA	2:C:72[A]:ILE:O	2.18	0.43
1:A:82:ASP:C	1:A:82:ASP:OD2	2.62	0.42
2:C:80:TYR:HE2	3:F:74:MET:O	2.02	0.42
3:D:181:CYS:HA	3:D:196:CYS:HA	2.01	0.42
1:B:210:GLN:NE2	2:E:44:THR:HG21	2.32	0.42
1:A:48:LYS:HD2	1:A:62:HIS:NE2	2.35	0.42
1:B:100:LEU:HD23	1:B:100:LEU:HA	1.83	0.42
1:A:206:MET:HE1	1:A:218:PHE:CE2	2.55	0.42
1:A:68:PRO:HG2	5:A:402:HEC:HBA1	2.02	0.41
2:E:75:ARG:HD2	10:E:261:HOH:O	2.18	0.41
3:D:218[A]:GLU:HG3	3:D:219:VAL:O	2.20	0.41
3:D:295:TYR:CD1	3:D:295:TYR:N	2.88	0.41
2:C:18:ASN:O	3:F:16:GLN:HA	2.20	0.41
1:A:43:ASP:HA	1:A:44:PRO:HD2	1.82	0.41
2:C:57[A]:OAF:HE3	2:C:108[A]:TRP:CG	2.55	0.41
1:B:202:ARG:HB2	1:B:206:MET:HG3	2.03	0.41
3:D:104:ARG:CG	3:D:105:GLY:N	2.83	0.41
1:A:199:TRP:HH2	1:A:333:MET:O	2.03	0.41
2:C:19:ASP:O	2:C:25:TYR:HB2	2.20	0.41
3:D:178:VAL:HG21	3:D:194:MET:HE1	2.03	0.41
2:E:56:SER:HB2	2:E:74:TYR:O	2.21	0.41
3:F:181[B]:CYS:HB3	3:F:196:CYS:HA	2.02	0.41
3:F:354:LYS:HE3	3:F:375:HIS:O	2.21	0.41
2:C:14:VAL:HA	2:C:15:PRO:HD2	1.81	0.41
3:D:153:PHE:CZ	3:D:163:GLY:HA3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ALA:HA	10:A:532:HOH:O	2.21	0.40
3:D:89:GLY:HA2	10:D:592:HOH:O	2.21	0.40
3:D:276:GLY:O	3:D:300:GLN:HA	2.21	0.40
3:F:88:ASP:OD1	3:F:88:ASP:C	2.64	0.40
2:E:91:THR:HB	3:F:306:HIS:CE1	2.56	0.40
3:F:54:HIS:O	3:F:55:PHE:HB2	2.22	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	355/373 (95%)	346 (98%)	9 (2%)	0	100	100
1	B	358/373 (96%)	350 (98%)	8 (2%)	0	100	100
2	C	129/137 (94%)	124 (96%)	3 (2%)	2 (2%)	7	4
2	E	126/137 (92%)	120 (95%)	6 (5%)	0	100	100
3	D	377/385 (98%)	361 (96%)	15 (4%)	1 (0%)	36	36
3	F	378/385 (98%)	362 (96%)	14 (4%)	2 (0%)	24	22
All	All	1723/1790 (96%)	1663 (96%)	55 (3%)	5 (0%)	36	36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	131	SER
3	F	32	ASP
2	C	130	ALA
3	F	102	ILE
3	D	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	279/292 (96%)	261 (94%)	18 (6%)	15	13
1	B	282/292 (97%)	272 (96%)	10 (4%)	32	35
2	C	111/112 (99%)	109 (98%)	2 (2%)	51	60
2	E	107/112 (96%)	104 (97%)	3 (3%)	38	43
3	D	307/310 (99%)	291 (95%)	16 (5%)	21	20
3	F	308/310 (99%)	303 (98%)	5 (2%)	55	64
All	All	1394/1428 (98%)	1340 (96%)	54 (4%)	31	31

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	8	ASP
1	A	39	ARG
1	A	51	LEU
1	A	84	ASN
1	A	112	VAL
1	A	157	GLU
1	A	190	GLU
1	A	201	CYS
1	A	202[A]	ARG
1	A	202[B]	ARG
1	A	206	MET
1	A	214	GLU
1	A	303[A]	GLU
1	A	303[B]	GLU
1	A	323	LEU
1	A	333	MET
1	A	358	LEU
1	B	8[A]	ASP
1	B	8[B]	ASP
1	B	60	GLN
1	B	157	GLU

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Mol	Chain	Res	Type
1	B	167	GLU
1	B	183	GLU
1	B	219	THR
1	B	285	THR
1	B	357	LEU
1	B	358	LEU
2	C	71	LEU
2	C	131	SER
3	D	20[A]	ARG
3	D	20[B]	ARG
3	D	45	ARG
3	D	92	ILE
3	D	117	VAL
3	D	127	LEU
3	D	177	ASP
3	D	211	THR
3	D	218[A]	GLU
3	D	218[B]	GLU
3	D	223	GLU
3	D	224	ASP
3	D	265	VAL
3	D	316	LEU
3	D	322	GLU
3	D	354	LYS
2	E	7	THR
2	E	58	VAL
2	E	71	LEU
3	F	11	GLN
3	F	75	ILE
3	F	160	PRO
3	F	262	LEU
3	F	343	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	60	GLN
1	A	62	HIS
1	A	84	ASN
1	A	210	GLN
1	B	16	GLN
1	B	210	GLN

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Mol	Chain	Res	Type
1	B	329	GLN
2	C	21	GLN
3	D	14	GLN
3	D	375	HIS
2	E	68	GLN
3	F	30	GLN
3	F	54	HIS
3	F	60	GLN
3	F	61	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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
2	0AF	C	57[B]	2	15,16,17	1.99	5 (33%)	14,22,24	1.34	2 (14%)
2	0AF	E	57[B]	2	15,16,17	2.23	5 (33%)	14,22,24	1.72	4 (28%)
2	0AF	C	57[A]	2	15,16,17	1.18	2 (13%)	14,22,24	1.13	1 (7%)
2	0AF	E	57[A]	2	15,16,17	1.23	1 (6%)	14,22,24	1.20	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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	0AF	C	57[B]	2	-	0/5/6/8	0/2/2/2
2	0AF	E	57[B]	2	-	0/5/6/8	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	0AF	C	57[A]	2	-	1/5/6/8	0/2/2/2
2	0AF	E	57[A]	2	-	0/5/6/8	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	57[B]	0AF	CD1-NE1	-4.69	1.29	1.37
2	E	57[B]	0AF	CE2-NE1	-4.59	1.30	1.37
2	C	57[B]	0AF	CE2-NE1	-4.16	1.30	1.37
2	C	57[B]	0AF	CD1-NE1	-3.76	1.31	1.37
2	E	57[B]	0AF	CD2-CE2	-2.85	1.37	1.41
2	C	57[B]	0AF	CD2-CE2	-2.80	1.37	1.41
2	C	57[A]	0AF	CD2-CE2	-2.57	1.38	1.41
2	E	57[A]	0AF	CD2-CE2	-2.54	1.38	1.41
2	C	57[B]	0AF	CD2-CG	-2.31	1.40	1.44
2	C	57[B]	0AF	CA-N	-2.27	1.41	1.48
2	E	57[B]	0AF	CE2-CZ2	-2.22	1.35	1.40
2	E	57[B]	0AF	CD2-CG	-2.20	1.40	1.44
2	C	57[A]	0AF	CD2-CG	-2.01	1.40	1.44

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	57[B]	0AF	CD2-CE2-NE1	3.27	112.19	107.54
2	E	57[B]	0AF	CB-CG-CD1	-2.82	121.47	126.97
2	C	57[B]	0AF	CB-CG-CD1	-2.74	121.62	126.97
2	C	57[A]	0AF	CG-CD1-NE1	-2.73	107.31	110.31
2	E	57[B]	0AF	CE3-CD2-CG	2.67	137.83	133.85
2	E	57[B]	0AF	CB-CG-CD2	2.32	131.16	126.70
2	C	57[B]	0AF	CB-CG-CD2	2.29	131.10	126.70

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	57[A]	0AF	C-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	57[B]	0AF	4	0
2	E	57[B]	0AF	2	0
2	C	57[A]	0AF	3	0
2	E	57[A]	0AF	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 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	$\# Z > 2$
9	PGE	F	402	-	9,9,9	0.51	0	8,8,8	0.41	0
5	HEC	A	403	1	46,50,50	2.50	19 (41%)	58,82,82	2.87	20 (34%)
5	HEC	B	402	1	46,50,50	2.51	20 (43%)	58,82,82	2.52	22 (37%)
6	ACT	D	401	-	3,3,3	0.88	0	3,3,3	1.04	0
6	ACT	A	407	-	3,3,3	0.86	0	3,3,3	1.51	0
5	HEC	A	402	1,10	46,50,50	2.65	22 (47%)	58,82,82	2.43	21 (36%)
6	ACT	A	404	-	3,3,3	0.87	0	3,3,3	1.55	1 (33%)
5	HEC	B	403	1	46,50,50	2.60	18 (39%)	58,82,82	2.86	21 (36%)
6	ACT	F	401	-	3,3,3	0.72	0	3,3,3	1.88	1 (33%)
8	EDO	B	405	-	3,3,3	0.52	0	2,2,2	0.07	0
6	ACT	B	404	-	3,3,3	0.97	0	3,3,3	1.78	1 (33%)

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
9	PGE	F	402	-	-	5/7/7/7	-
5	HEC	A	403	1	-	6/14/54/54	-
5	HEC	B	402	1	-	7/14/54/54	-
5	HEC	A	402	1,10	-	6/14/54/54	-
5	HEC	B	403	1	-	6/14/54/54	-
8	EDO	B	405	-	-	1/1/1/1	-

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	403	HEC	CHB-C4A	6.36	1.50	1.38
5	A	402	HEC	CAC-C3C	5.74	1.53	1.35
5	A	403	HEC	CAC-C3C	5.49	1.52	1.35
5	A	402	HEC	CAB-C3B	5.27	1.52	1.35
5	B	403	HEC	C4C-NC	-5.25	1.29	1.39
5	B	403	HEC	CAC-C3C	5.23	1.52	1.35
5	A	403	HEC	CAB-C3B	5.13	1.51	1.35
5	B	403	HEC	C4D-ND	-5.08	1.30	1.39
5	B	403	HEC	CAB-C3B	4.89	1.50	1.35
5	B	402	HEC	CAB-C3B	4.88	1.50	1.35
5	B	402	HEC	CHB-C4A	4.75	1.47	1.38
5	B	402	HEC	C4A-NA	-4.61	1.30	1.39
5	B	402	HEC	CAC-C3C	4.59	1.49	1.35
5	A	402	HEC	CHD-C1D	4.55	1.49	1.39
5	A	402	HEC	CHA-C1A	4.51	1.47	1.38
5	A	402	HEC	CHC-C4B	4.48	1.47	1.38
5	A	403	HEC	C4A-NA	-4.44	1.31	1.39
5	A	403	HEC	CHB-C4A	4.37	1.47	1.38
5	B	402	HEC	C1C-NC	-4.35	1.31	1.39
5	A	403	HEC	CHC-C4B	4.26	1.46	1.38
5	B	403	HEC	C4A-NA	-4.25	1.31	1.39
5	A	403	HEC	C4D-ND	-4.24	1.31	1.39
5	B	402	HEC	CHD-C4C	4.19	1.46	1.38
5	A	402	HEC	C1D-ND	-4.17	1.31	1.39
5	A	403	HEC	CHA-C1A	4.11	1.46	1.38
5	A	402	HEC	CHC-C1C	4.07	1.48	1.39
5	B	403	HEC	C1D-ND	-3.95	1.32	1.39
5	B	402	HEC	C1D-ND	-3.93	1.32	1.39
5	A	403	HEC	C1A-NA	-3.93	1.32	1.39
5	A	403	HEC	CHD-C4C	3.92	1.46	1.38
5	B	403	HEC	CHC-C4B	3.90	1.46	1.38
5	A	402	HEC	CHB-C4A	3.87	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	403	HEC	CHD-C4C	3.78	1.45	1.38
5	B	402	HEC	C4C-NC	-3.75	1.32	1.39
5	A	403	HEC	C4B-NB	-3.67	1.32	1.39
5	B	402	HEC	CHA-C1A	3.56	1.45	1.38
5	A	402	HEC	CHB-C1B	3.45	1.47	1.39
5	B	402	HEC	CHC-C4B	3.42	1.45	1.38
5	A	402	HEC	CHA-C4D	3.39	1.47	1.39
5	A	402	HEC	C1C-NC	-3.36	1.33	1.39
5	A	402	HEC	CHD-C4C	3.35	1.44	1.38
5	B	402	HEC	CHD-C1D	3.32	1.46	1.39
5	A	403	HEC	C1B-NB	-3.32	1.33	1.39
5	B	403	HEC	C4B-NB	-3.31	1.33	1.39
5	A	402	HEC	C1A-NA	-3.29	1.33	1.39
5	A	402	HEC	C4D-ND	-3.29	1.33	1.39
5	A	402	HEC	C1B-NB	-3.27	1.33	1.39
5	B	402	HEC	C1B-NB	-3.23	1.33	1.39
5	B	402	HEC	CHC-C1C	3.22	1.46	1.39
5	A	403	HEC	CHD-C1D	3.12	1.46	1.39
5	A	402	HEC	C4C-NC	-3.11	1.33	1.39
5	A	402	HEC	C1A-C2A	3.10	1.50	1.45
5	B	403	HEC	CHC-C1C	3.08	1.46	1.39
5	B	402	HEC	CHB-C1B	2.99	1.46	1.39
5	A	403	HEC	C4C-NC	-2.95	1.34	1.39
5	B	402	HEC	CHA-C4D	2.90	1.45	1.39
5	A	403	HEC	CHA-C4D	2.86	1.45	1.39
5	B	402	HEC	C4B-NB	-2.81	1.34	1.39
5	B	403	HEC	CHA-C1A	2.81	1.43	1.38
5	B	403	HEC	C1A-NA	-2.80	1.34	1.39
5	A	403	HEC	CHB-C1B	2.80	1.45	1.39
5	A	403	HEC	CHC-C1C	2.78	1.45	1.39
5	A	402	HEC	C4A-NA	-2.62	1.34	1.39
5	B	403	HEC	CHA-C4D	2.62	1.45	1.39
5	B	402	HEC	C1D-C2D	2.52	1.49	1.43
5	B	403	HEC	C4A-C3A	2.42	1.50	1.45
5	B	403	HEC	CHB-C1B	2.41	1.44	1.39
5	B	403	HEC	C1B-NB	-2.40	1.35	1.39
5	A	403	HEC	C1C-NC	-2.39	1.35	1.39
5	B	403	HEC	C1B-C2B	2.38	1.48	1.43
5	A	402	HEC	C4B-NB	-2.36	1.35	1.39
5	A	403	HEC	C4A-C3A	2.35	1.50	1.45
5	A	402	HEC	C1B-C2B	2.34	1.48	1.43
5	A	403	HEC	C1D-C2D	2.32	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	402	HEC	C4A-C3A	2.24	1.49	1.45
5	A	402	HEC	C4A-C3A	2.22	1.49	1.45
5	B	402	HEC	C3B-C4B	2.13	1.49	1.46
5	A	402	HEC	C1D-C2D	2.11	1.48	1.43
5	B	402	HEC	C4D-ND	-2.04	1.35	1.39

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	403	HEC	CBB-CAB-C3B	-13.84	99.77	127.43
5	A	403	HEC	CBB-CAB-C3B	-13.35	100.75	127.43
5	B	402	HEC	CBB-CAB-C3B	-10.01	107.43	127.43
5	A	402	HEC	CBB-CAB-C3B	-8.91	109.62	127.43
5	A	403	HEC	CBC-CAC-C3C	-8.04	111.37	127.43
5	B	403	HEC	CBC-CAC-C3C	-7.35	112.75	127.43
5	B	402	HEC	CBC-CAC-C3C	-6.80	113.85	127.43
5	A	402	HEC	CBC-CAC-C3C	-6.69	114.06	127.43
5	B	403	HEC	C2A-C1A-NA	6.19	116.30	110.32
5	A	403	HEC	CBD-CAD-C3D	-5.50	97.32	112.53
5	B	402	HEC	C3D-C4D-ND	4.86	115.55	110.15
5	A	403	HEC	C1D-C2D-C3D	-4.30	101.89	106.82
5	B	403	HEC	CBD-CAD-C3D	-4.26	100.75	112.53
5	A	402	HEC	C3D-C4D-ND	4.24	114.86	110.15
5	B	403	HEC	C1A-C2A-C3A	-4.03	101.80	107.11
5	B	402	HEC	C2A-C1A-NA	3.93	114.11	110.32
5	A	403	HEC	C2A-C1A-NA	3.92	114.11	110.32
5	A	403	HEC	C3D-C4D-ND	3.88	114.45	110.15
5	A	402	HEC	CHD-C4C-NC	-3.73	120.39	124.45
5	A	402	HEC	CBD-CAD-C3D	-3.69	102.33	112.53
5	B	403	HEC	CHB-C4A-NA	-3.59	120.55	124.45
5	B	402	HEC	CBD-CAD-C3D	-3.55	102.71	112.53
5	B	402	HEC	CHC-C4B-NB	-3.52	120.61	124.45
5	A	403	HEC	CHB-C4A-NA	-3.52	120.62	124.45
5	A	402	HEC	C2A-C1A-NA	3.47	113.68	110.32
5	A	402	HEC	C2B-C1B-NB	3.45	115.67	110.14
5	B	403	HEC	C1D-C2D-C3D	-3.41	102.91	106.82
5	A	403	HEC	CBA-CAA-C2A	-3.27	103.50	112.53
5	B	402	HEC	C1A-C2A-C3A	-3.20	102.89	107.11
5	A	403	HEC	CMB-C2B-C3B	3.17	134.01	126.55
5	B	402	HEC	C2B-C1B-NB	3.07	115.06	110.14
5	A	403	HEC	CHD-C4C-NC	-3.05	121.13	124.45
5	B	402	HEC	CMB-C2B-C3B	3.03	133.67	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	402	HEC	C4D-C3D-C2D	-2.94	102.32	106.87
5	A	402	HEC	C2D-C1D-ND	2.92	114.82	110.14
5	B	403	HEC	C2D-C1D-ND	2.89	114.77	110.14
5	B	403	HEC	CHA-C1A-NA	-2.88	121.32	124.45
5	B	402	HEC	CMC-C2C-C3C	2.84	133.23	126.55
5	A	403	HEC	CHA-C1A-C2A	-2.75	120.52	124.86
5	A	402	HEC	C3A-C4A-NA	2.73	114.69	109.64
5	A	403	HEC	CAA-C2A-C3A	2.72	132.95	127.87
5	B	403	HEC	CBA-CAA-C2A	-2.71	105.04	112.53
5	A	403	HEC	C4A-C3A-C2A	-2.71	102.95	106.97
5	A	403	HEC	C2D-C1D-ND	2.70	114.48	110.14
5	B	402	HEC	CHD-C4C-NC	-2.67	121.55	124.45
5	A	402	HEC	C4A-C3A-C2A	-2.66	103.03	106.97
5	B	403	HEC	CMB-C2B-C3B	2.61	132.70	126.55
5	A	403	HEC	C2B-C1B-NB	2.61	114.33	110.14
5	A	402	HEC	CAA-CBA-CGA	-2.59	106.81	113.67
5	B	403	HEC	C3A-C4A-NA	2.54	114.33	109.64
5	B	402	HEC	C2C-C1C-NC	2.54	114.21	110.14
5	B	402	HEC	O2D-CGD-CBD	2.53	122.00	114.00
6	F	401	ACT	OXT-C-CH3	2.53	125.65	115.05
5	A	402	HEC	C4D-C3D-C2D	-2.52	102.97	106.87
5	B	402	HEC	O1D-CGD-CBD	-2.51	115.13	123.09
5	A	402	HEC	C1D-C2D-C3D	-2.50	103.95	106.82
5	A	402	HEC	C2C-C1C-NC	2.50	114.14	110.14
5	B	402	HEC	CBA-CAA-C2A	-2.49	105.65	112.53
5	A	403	HEC	C2C-C1C-NC	2.47	114.11	110.14
5	B	403	HEC	CAD-CBD-CGD	-2.47	107.12	113.67
5	B	403	HEC	CHC-C1C-C2C	-2.42	120.39	127.43
5	A	402	HEC	CHA-C1A-NA	-2.40	121.84	124.45
5	B	403	HEC	C2B-C1B-NB	2.38	113.96	110.14
5	B	402	HEC	C2D-C1D-ND	2.38	113.95	110.14
6	B	404	ACT	OXT-C-O	-2.36	113.28	122.03
5	A	402	HEC	CMB-C2B-C3B	2.36	132.09	126.55
5	B	403	HEC	CHD-C1D-C2D	-2.34	120.64	127.43
5	B	402	HEC	CAA-C2A-C1A	2.33	129.59	124.85
5	A	402	HEC	CMC-C2C-C3C	2.32	132.01	126.55
5	B	402	HEC	CMB-C2B-C1B	-2.29	121.94	125.42
5	A	402	HEC	CAA-C2A-C1A	2.28	129.49	124.85
5	B	402	HEC	C1D-C2D-C3D	-2.26	104.23	106.82
5	A	403	HEC	C1A-C2A-C3A	-2.26	104.14	107.11
5	A	403	HEC	CMD-C2D-C1D	2.21	128.78	125.42
5	A	403	HEC	CMA-C3A-C4A	2.20	128.60	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	402	HEC	CHC-C1C-C2C	-2.20	121.05	127.43
5	B	403	HEC	C2C-C1C-NC	2.19	113.65	110.14
5	B	403	HEC	CAD-C3D-C4D	2.18	129.20	124.94
5	B	402	HEC	O2A-CGA-CBA	2.17	120.87	114.00
5	A	402	HEC	CHD-C1D-ND	-2.15	119.96	123.86
5	A	402	HEC	C4B-NB-C1B	-2.09	102.42	105.82
5	B	403	HEC	C3D-C4D-ND	2.08	112.46	110.15
5	B	403	HEC	C4A-NA-C1A	-2.07	102.45	105.82
5	B	403	HEC	CMD-C2D-C3D	2.06	130.00	125.62
5	A	403	HEC	C3A-C4A-NA	2.02	113.37	109.64
5	B	402	HEC	CHB-C4A-NA	-2.02	122.26	124.45
6	A	404	ACT	OXT-C-O	-2.01	114.56	122.03

There are no chirality outliers.

All (31) 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
5	B	403	HEC	C2B-C3B-CAB-CBB
5	B	403	HEC	C2C-C3C-CAC-CBC
5	B	403	HEC	C4C-C3C-CAC-CBC
8	B	405	EDO	O1-C1-C2-O2
9	F	402	PGE	O2-C3-C4-O3
9	F	402	PGE	O3-C5-C6-O4
9	F	402	PGE	C3-C4-O3-C5
5	B	403	HEC	C4B-C3B-CAB-CBB
9	F	402	PGE	C1-C2-O2-C3
9	F	402	PGE	O1-C1-C2-O2
5	B	403	HEC	CAD-CBD-CGD-O2D
5	B	402	HEC	CAD-CBD-CGD-O2D
5	A	402	HEC	CAD-CBD-CGD-O2D

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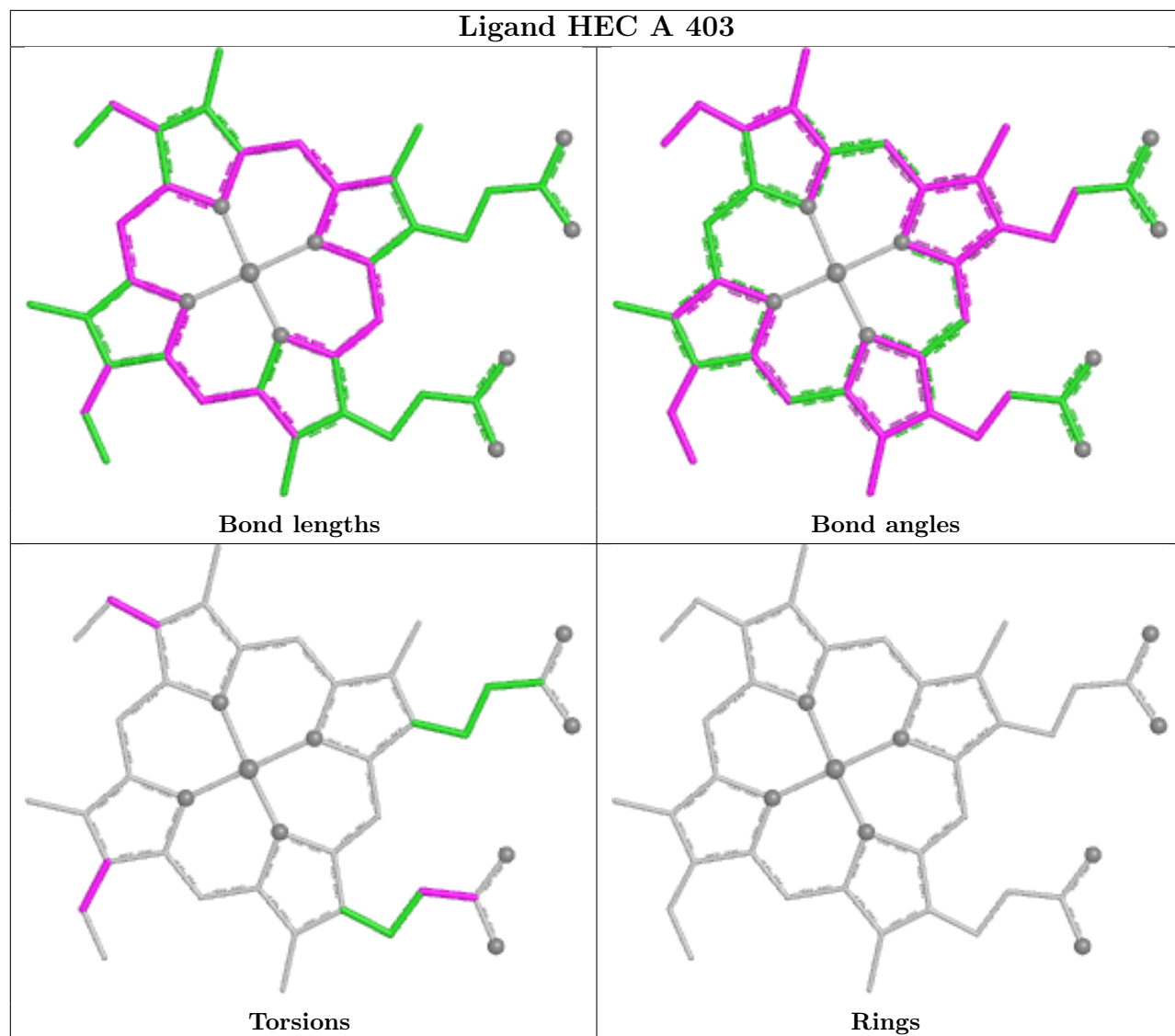
Mol	Chain	Res	Type	Atoms
5	A	402	HEC	CAD-CBD-CGD-O1D
5	A	403	HEC	CAD-CBD-CGD-O2D
5	B	403	HEC	CAD-CBD-CGD-O1D
5	A	403	HEC	CAD-CBD-CGD-O1D
5	B	402	HEC	CAD-CBD-CGD-O1D
5	B	402	HEC	CAA-CBA-CGA-O2A

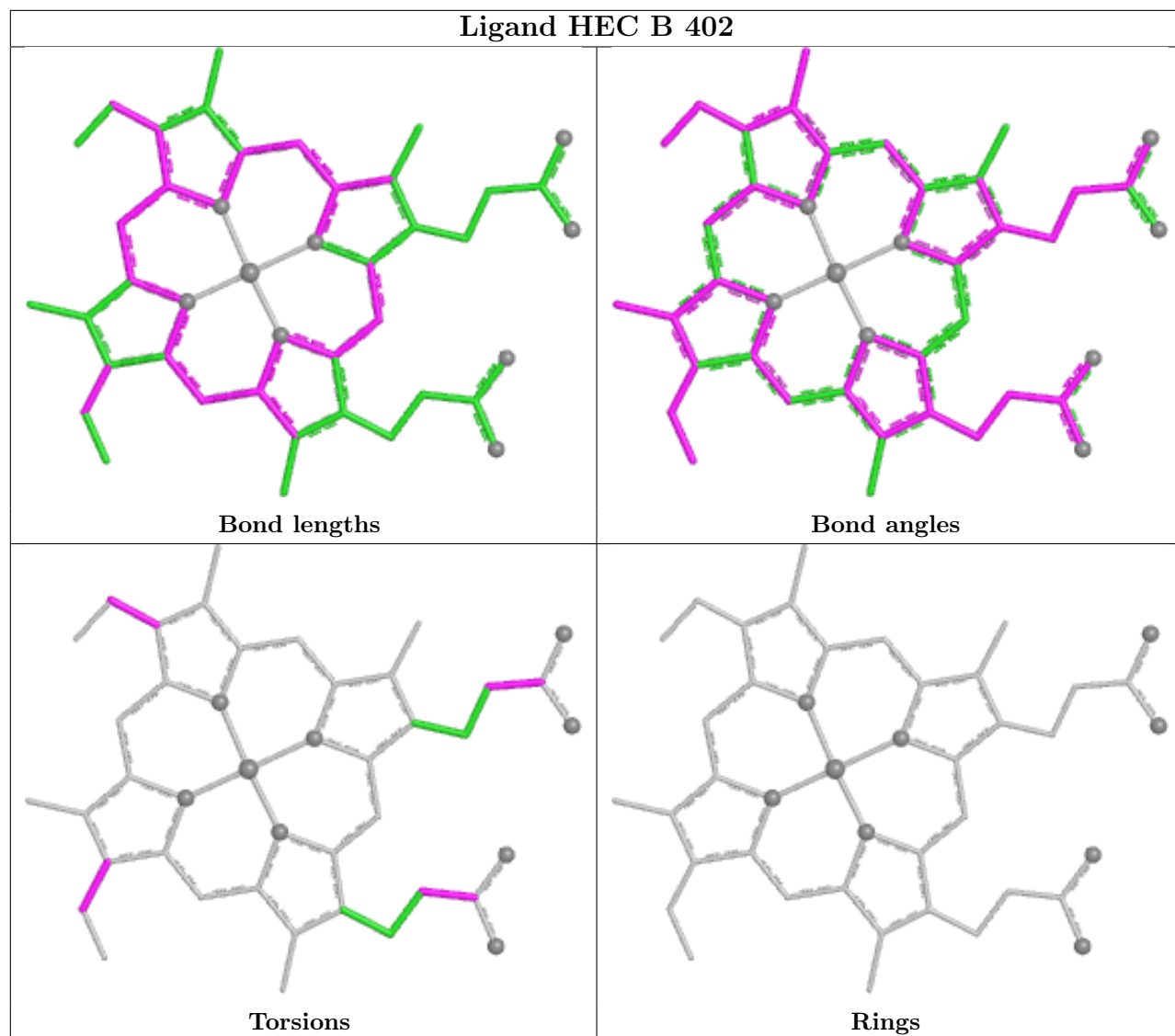
There are no ring outliers.

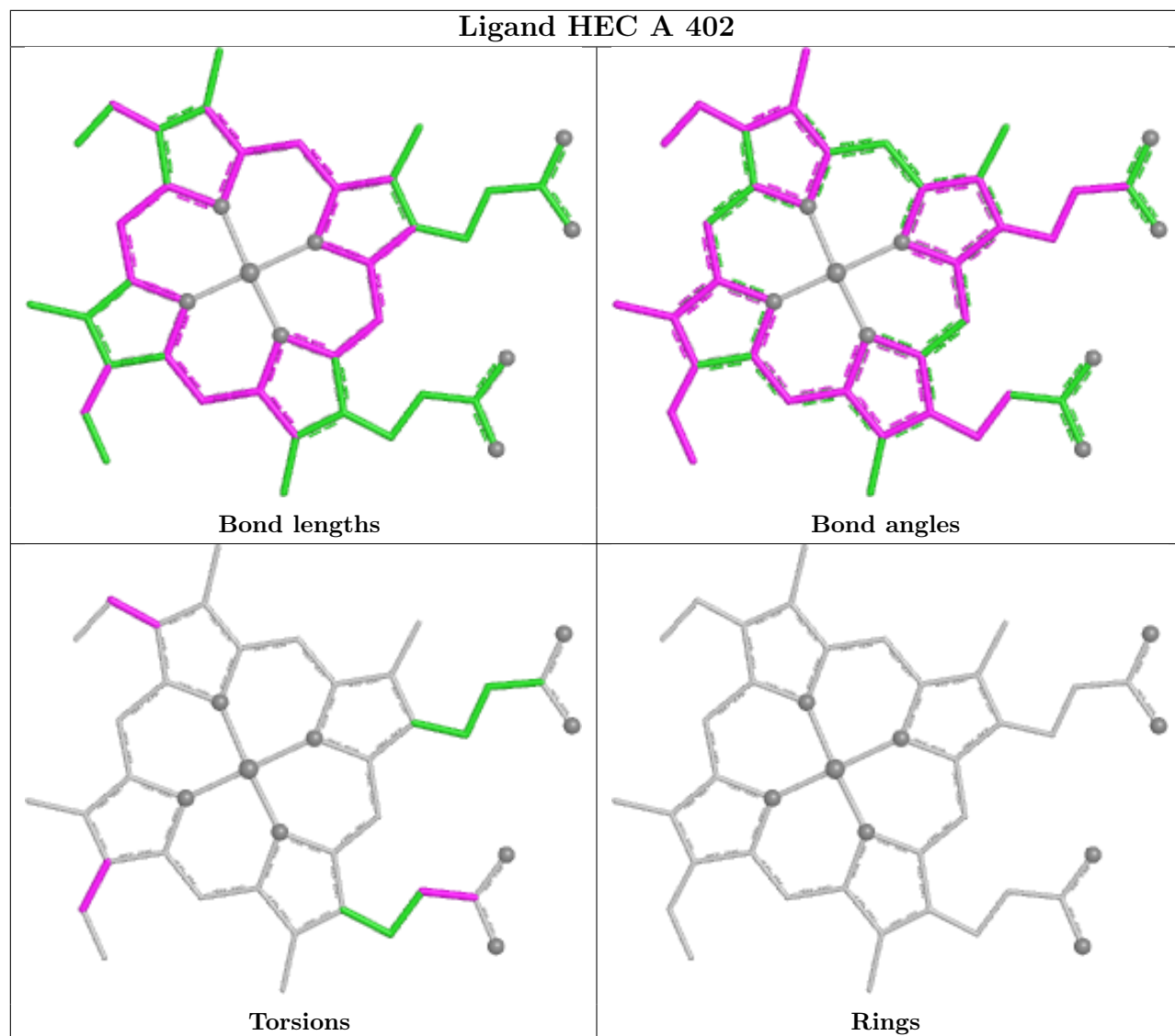
3 monomers are involved in 3 short contacts:

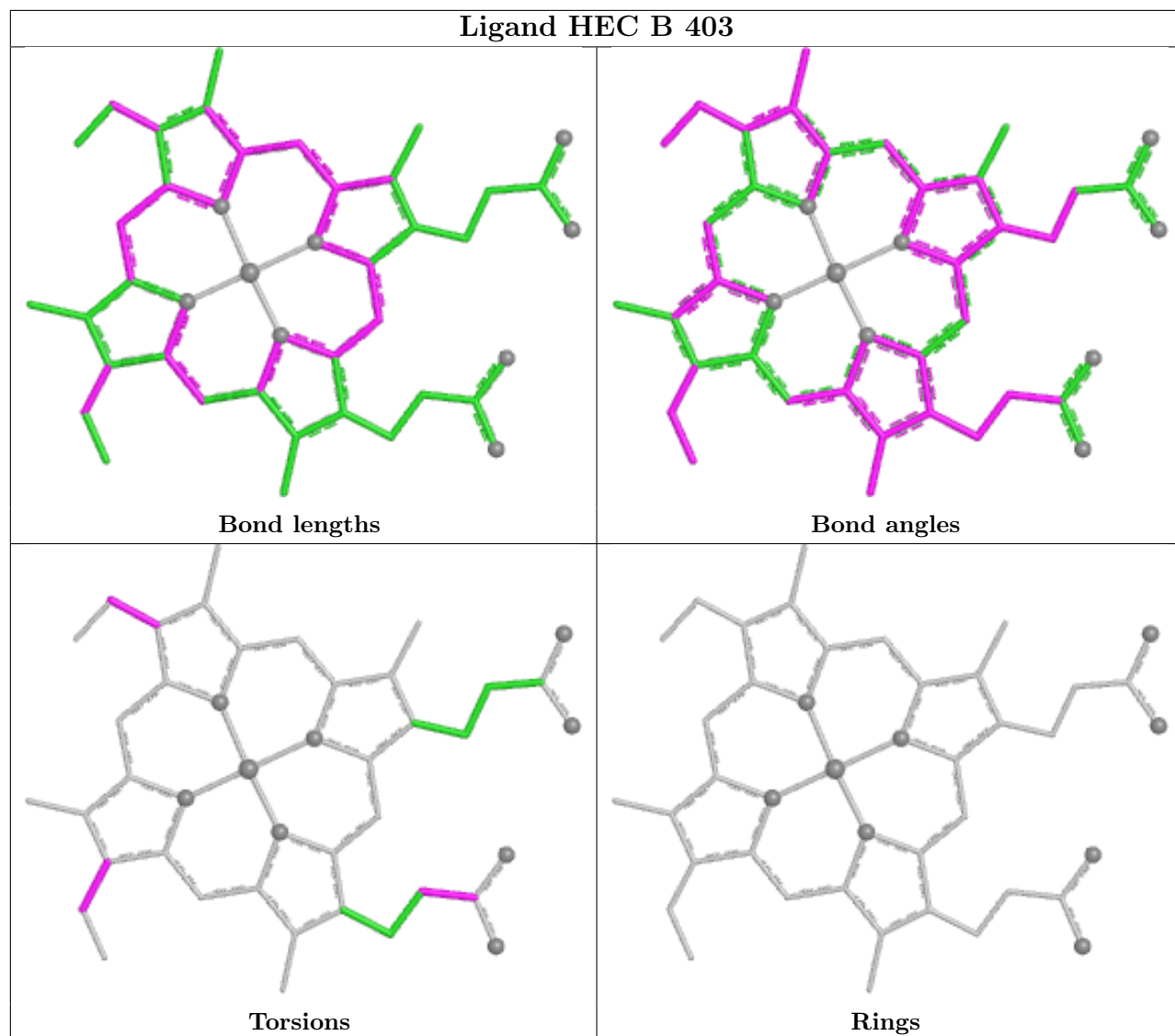
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	F	402	PGE	1	0
5	B	402	HEC	1	0
5	A	402	HEC	1	0

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 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%)	-0.34	0 100 100	19, 42, 59, 74	3 (0%)
1	B	357/373 (95%)	-0.54	1 (0%) 90 91	17, 35, 53, 80	3 (0%)
2	C	128/137 (93%)	-0.23	2 (1%) 70 73	19, 38, 64, 95	3 (2%)
2	E	125/137 (91%)	-0.60	2 (1%) 70 73	14, 30, 45, 68	3 (2%)
3	D	376/385 (97%)	-0.25	1 (0%) 90 91	19, 44, 70, 84	3 (0%)
3	F	376/385 (97%)	-0.65	0 100 100	14, 32, 49, 68	4 (1%)
All	All	1716/1790 (95%)	-0.44	6 (0%) 90 91	14, 37, 61, 95	19 (1%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	ALA	2.9
2	C	131	SER	2.7
3	D	207	GLY	2.2
2	E	131	SER	2.1
2	C	134	HIS	2.1
2	E	6	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, 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	0AF	C	57[A]	15/16	0.93	0.10	35,39,43,43	15
2	0AF	C	57[B]	15/16	0.93	0.10	44,51,55,55	15
2	0AF	E	57[A]	15/16	0.93	0.09	29,31,33,33	15

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	0AF	E	57[B]	15/16	0.93	0.09	32,36,40,45	15

6.3 Carbohydrates [i](#)

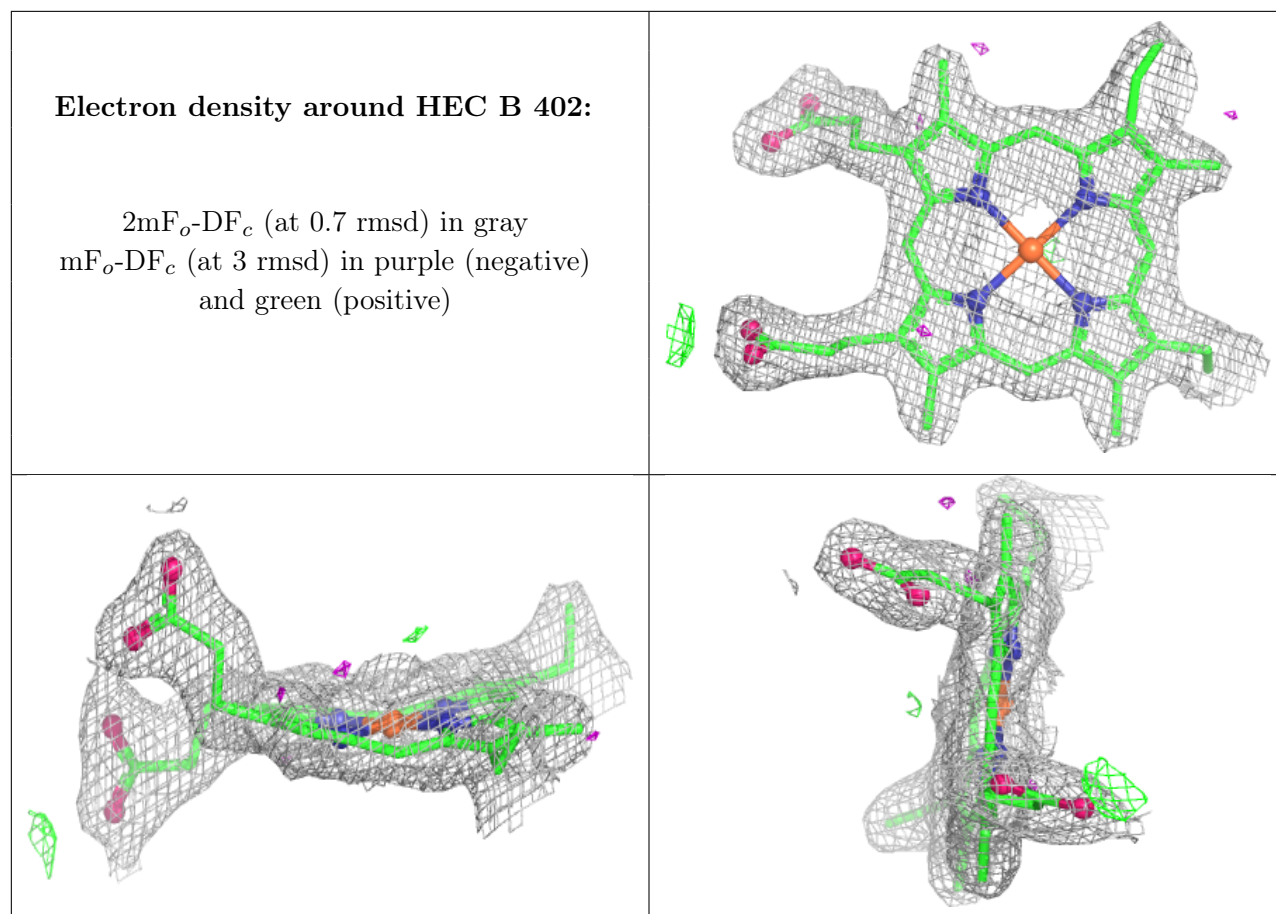
There are no oligosaccharides in this entry.

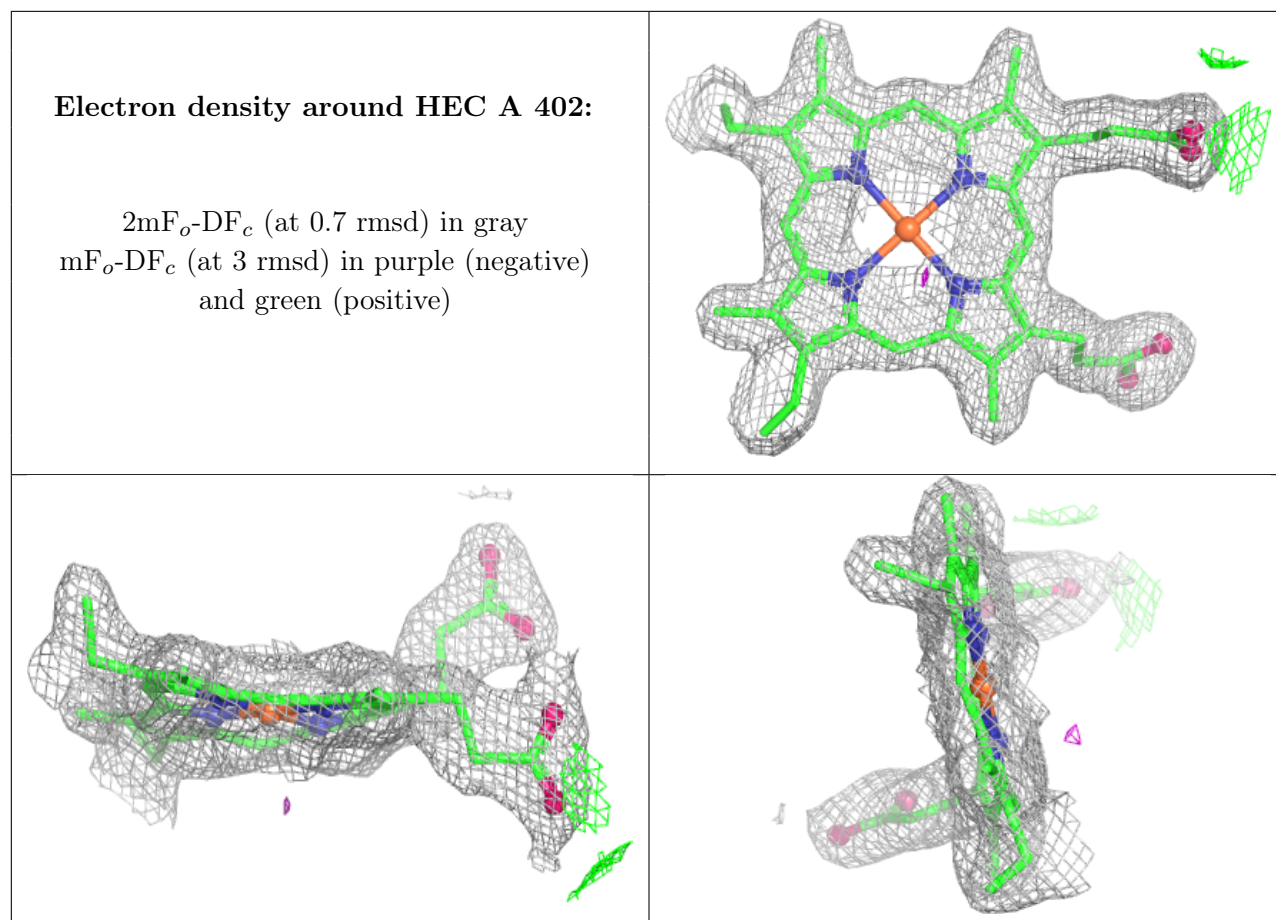
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
6	ACT	A	407	4/4	0.71	0.22	74,74,74,75	0
9	PGE	F	402	10/10	0.77	0.18	78,91,97,99	0
6	ACT	A	404	4/4	0.80	0.18	80,80,81,81	0
6	ACT	B	404	4/4	0.85	0.14	61,62,63,63	0
7	NA	A	405	1/1	0.86	0.17	55,55,55,55	0
7	NA	A	406	1/1	0.90	0.07	52,52,52,52	0
6	ACT	D	401	4/4	0.90	0.10	44,46,47,47	0
6	ACT	F	401	4/4	0.91	0.11	47,49,50,51	0
8	EDO	B	405	4/4	0.93	0.10	44,47,49,49	0
7	NA	B	407	1/1	0.96	0.05	38,38,38,38	0
7	NA	B	406	1/1	0.97	0.04	42,42,42,42	0
5	HEC	B	402	43/43	0.98	0.05	23,30,34,35	0
5	HEC	A	402	43/43	0.98	0.06	28,34,37,39	0
5	HEC	B	403	43/43	0.99	0.05	19,24,29,34	0
5	HEC	A	403	43/43	0.99	0.05	27,33,36,37	0
4	CA	A	401	1/1	0.99	0.02	34,34,34,34	0
4	CA	B	401	1/1	1.00	0.02	27,27,27,27	0

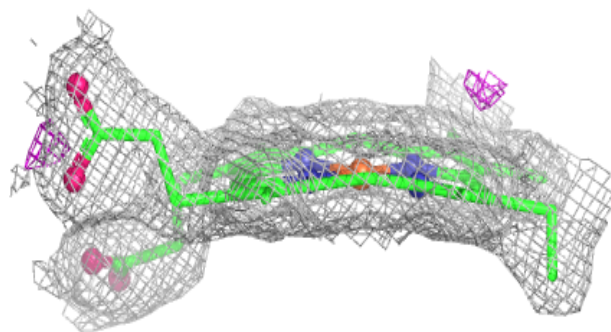
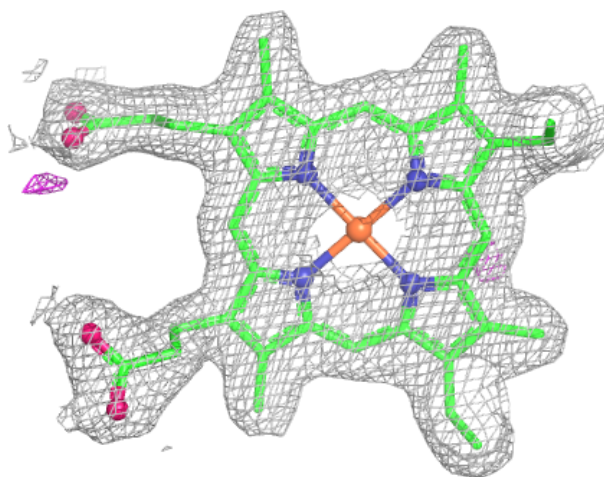
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

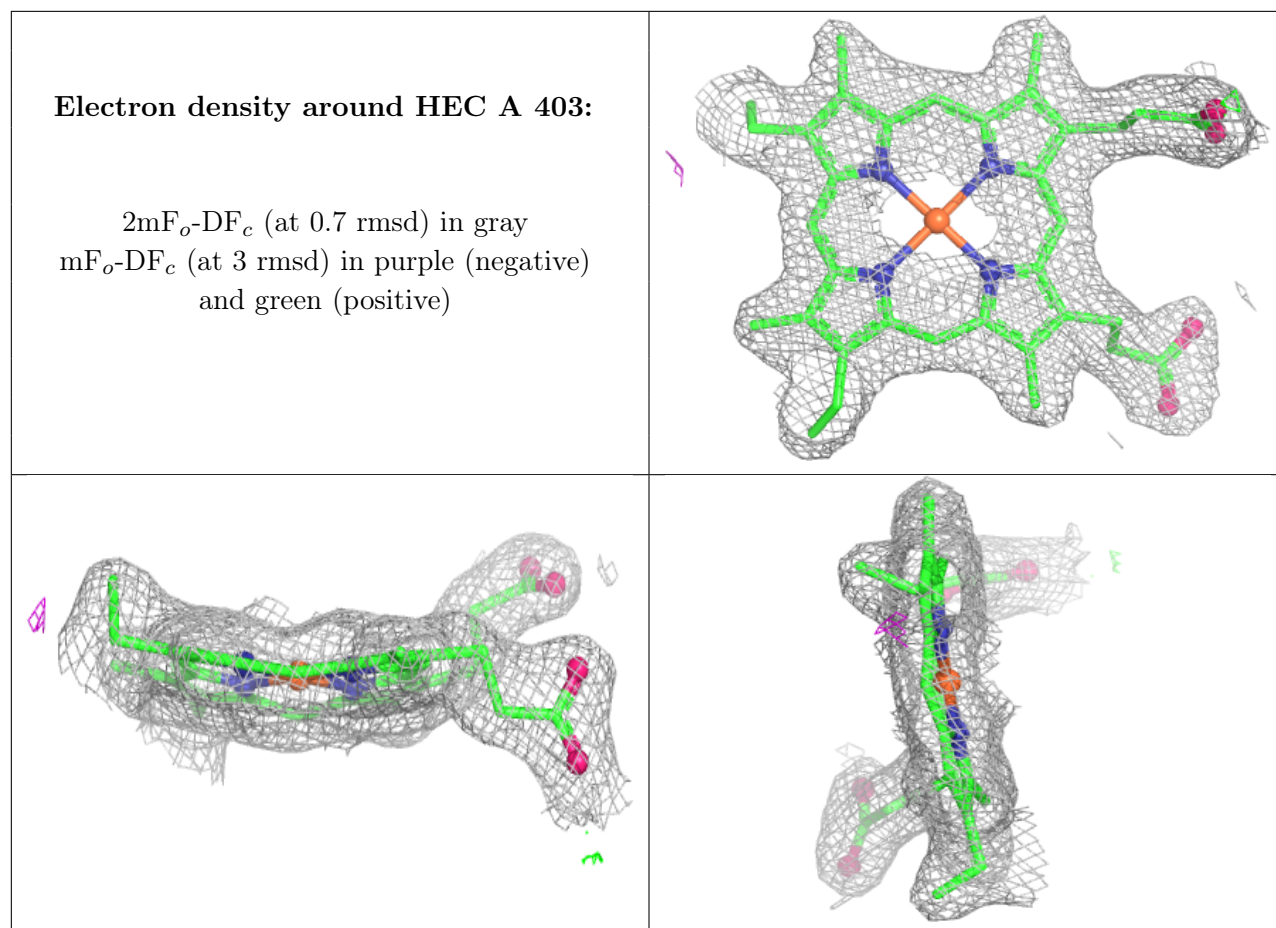




Electron density around HEC B 403:

$2mF_o-DF_c$ (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.