



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 8, 2024 – 12:13 PM EDT

PDB ID : 8VKD
Title : Crystal structure of dehaloperoxidase A in complex with substrate 4-nitrocatechol
Authors : Aktar, M.S.; de Serrano, V.S.; Ghiladi, R.A.; Franzen, S.
Deposited on : 2024-01-08
Resolution : 1.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.37.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

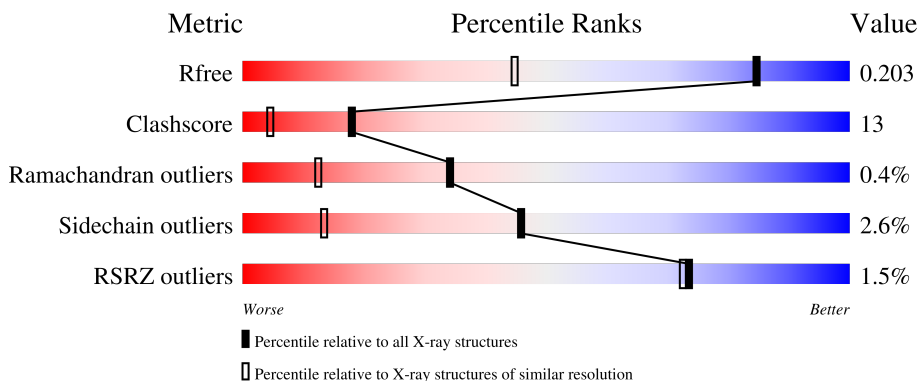
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


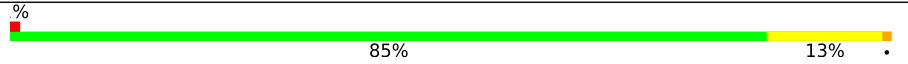
The reported resolution of this entry is 1.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	AAA	137	 82% 17% .
1	BBB	137	 85% 13% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PEG	AAA	203[A]	-	-	X	-
4	PEG	AAA	206	-	-	X	-
5	4NC	AAA	204	-	-	X	-
5	4NC	BBB	202	-	-	X	-
6	DMS	AAA	205	-	-	X	-

2 Entry composition [i](#)

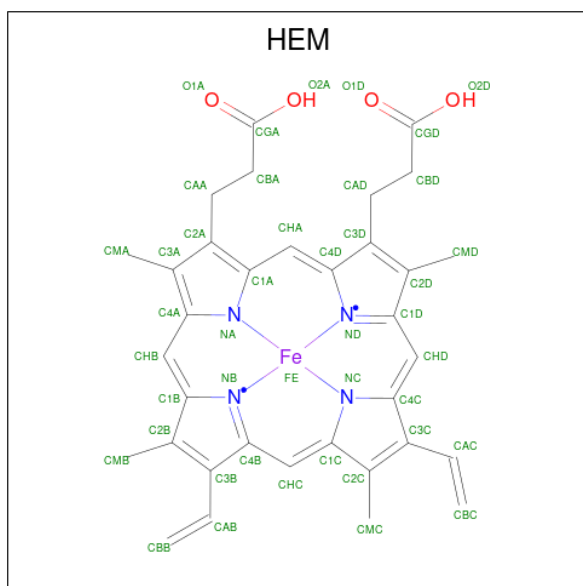
There are 8 unique types of molecules in this entry. The entry contains 2980 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dehaloperoxidase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	137	Total	C	N	O	S	0	28	0
			1334	824	241	261	8			
1	BBB	137	Total	C	N	O	S	0	25	0
			1284	797	224	256	7			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



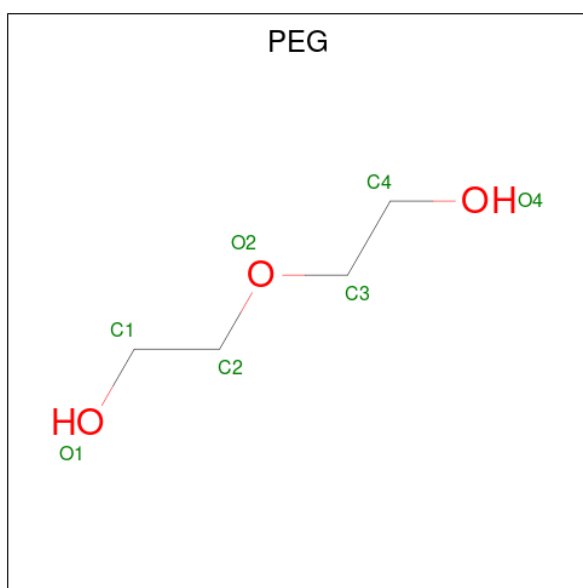
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
2	AAA	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	BBB	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



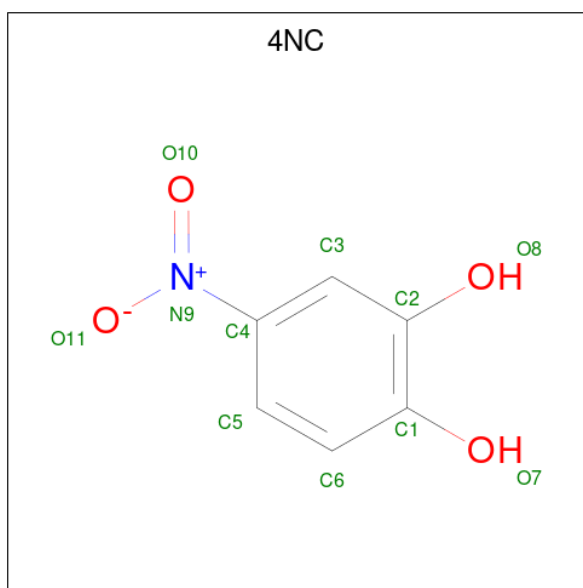
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	O	0	0
			6	3	3		
3	AAA	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



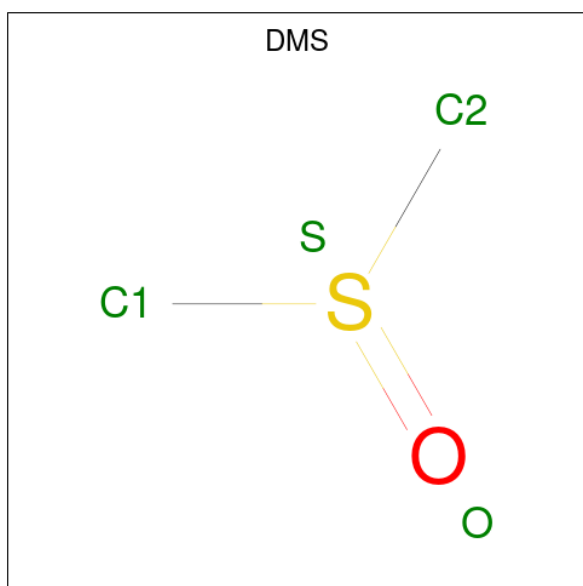
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	1
			14	8	6		
4	AAA	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is 4-NITROCATECHOL (three-letter code: 4NC) (formula: $C_6H_5NO_4$).



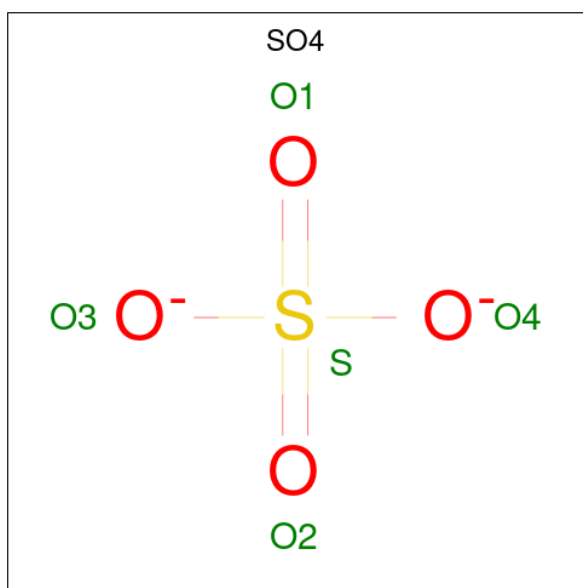
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	AAA	1	Total	C	N	O	0	0
			11	6	1	4		
5	BBB	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	AAA	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	1	Total O S 5 4 1	0	0
7	BBB	1	Total O S 5 4 1	0	0
7	BBB	1	Total O S 5 4 1	0	0


- Molecule 8 is water.

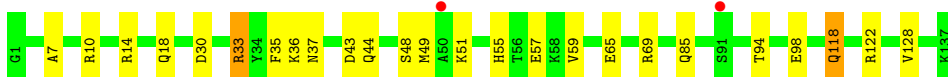
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	AAA	105	Total O 105 105	0	0
8	BBB	97	Total O 97 97	0	0

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Dehaloperoxidase A

Chain AAA:  82% 17%



- Molecule 1: Dehaloperoxidase A

Chain BBB:  85% 13%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.36Å 68.04Å 68.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.41 – 1.40 44.37 – 1.40	Depositor EDS
% Data completeness (in resolution range)	94.7 (44.41-1.40) 93.8 (44.37-1.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 1.40Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.166 , 0.201 0.172 , 0.203	Depositor DCC
R_{free} test set	2581 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	11.9	Xtrriage
Anisotropy	0.297	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.097 for -h,l,k	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2980	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.83% 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: SO4, 4NC, PEG, DMS, HEM, GOL

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	AAA	0.93	0/1355	0.95	0/1809
1	BBB	0.87	0/1314	0.95	1/1757 (0.1%)
All	All	0.90	0/2669	0.95	1/3566 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	5	ASP	CB-CG-OD2	-6.25	112.67	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	1334	0	1281	48	0
1	BBB	1284	0	1234	22	0
2	AAA	43	0	30	3	0
2	BBB	43	0	30	0	0
3	AAA	12	0	16	3	0
4	AAA	21	0	29	15	0
5	AAA	11	0	3	5	0
5	BBB	11	0	2	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AAA	4	0	6	5	0
7	AAA	5	0	0	0	0
7	BBB	10	0	0	0	0
8	AAA	105	0	0	9	0
8	BBB	97	0	0	7	0
All	All	2980	0	2631	74	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 13.

All (74) 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)
5:AAA:204:4NC:H5	8:AAA:317:HOH:O	1.13	1.24
1:AAA:55[B]:HIS:CD2	2:AAA:201:HEM:O1A	1.93	1.21
5:AAA:204:4NC:C5	8:AAA:317:HOH:O	1.68	1.20
5:BBB:202:4NC:H5	8:BBB:326:HOH:O	0.98	1.15
1:AAA:69:ARG:NH1	4:AAA:206:PEG:H32	1.78	0.99
5:BBB:202:4NC:C5	8:BBB:326:HOH:O	1.64	0.96
1:AAA:55[B]:HIS:HD2	2:AAA:201:HEM:O1A	1.34	0.91
1:AAA:122[B]:ARG:NH1	1:BBB:72[B]:ASP:OD1	2.05	0.90
1:AAA:30[A]:ASP:O	1:AAA:33[A]:ARG:HG2	1.73	0.88
1:BBB:54:ASP:HB3	8:BBB:380:HOH:O	1.72	0.88
1:AAA:55[A]:HIS:CG	5:AAA:204:4NC:O7	2.05	0.86
1:AAA:69:ARG:HH12	4:AAA:206:PEG:C3	1.88	0.86
1:AAA:69:ARG:HH12	4:AAA:206:PEG:H32	1.39	0.81
1:AAA:10[B]:ARG:NH2	1:AAA:65[B]:GLU:OE2	2.21	0.74
1:AAA:69:ARG:NH1	4:AAA:206:PEG:C3	2.49	0.73
1:BBB:22:LEU:HD11	1:BBB:47[A]:LYS:HD2	1.74	0.70
1:AAA:14[B]:ARG:HG2	1:AAA:57[B]:GLU:OE1	1.91	0.70
1:AAA:51:LYS:CB	8:AAA:397:HOH:O	2.40	0.69
1:AAA:51:LYS:HB3	8:AAA:397:HOH:O	1.92	0.68
1:AAA:14[A]:ARG:NH2	1:AAA:57[A]:GLU:OE1	2.29	0.65
1:AAA:10[A]:ARG:NH1	4:AAA:203[A]:PEG:O4	2.30	0.65
4:AAA:203[A]:PEG:H41	8:AAA:301:HOH:O	1.97	0.65
1:AAA:69:ARG:HH22	4:AAA:206:PEG:C1	2.12	0.63
1:AAA:49[B]:MET:HG2	8:AAA:333:HOH:O	2.00	0.62
1:BBB:98:GLU:HG2	1:BBB:128:VAL:HG21	1.84	0.59
1:AAA:94:THR:HB	1:AAA:128:VAL:HG13	1.86	0.57
1:BBB:13:LEU:HD22	1:BBB:57[A]:GLU:HG3	1.87	0.56
1:AAA:118[A]:GLN:HG3	3:AAA:207:GOL:O1	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:14[A]:ARG:NE	1:AAA:57[A]:GLU:OE1	2.36	0.55
1:AAA:118[A]:GLN:CG	3:AAA:207:GOL:O1	2.54	0.55
1:AAA:18:GLN:NE2	8:AAA:304:HOH:O	2.39	0.55
1:AAA:35:PHE:HE1	5:AAA:204:4NC:C6	2.21	0.54
1:AAA:44[B]:GLN:O	1:AAA:48[B]:SER:OG	2.14	0.54
1:BBB:43:ASP:O	1:BBB:47[A]:LYS:HD3	2.09	0.53
1:BBB:36:LYS:O	1:BBB:37:ASN:HB2	2.07	0.53
1:AAA:122[B]:ARG:NH1	1:BBB:72[B]:ASP:CG	2.63	0.52
1:AAA:14[A]:ARG:HH21	1:AAA:57[A]:GLU:CD	2.13	0.52
1:AAA:65[B]:GLU:OE1	4:AAA:206:PEG:H31	2.11	0.51
1:BBB:35:PHE:HE1	5:BBB:202:4NC:C6	2.22	0.51
1:BBB:94:THR:HB	1:BBB:128:VAL:HG13	1.92	0.50
1:AAA:69:ARG:HH12	4:AAA:206:PEG:H31	1.72	0.50
1:AAA:69:ARG:HH12	4:AAA:206:PEG:C1	2.25	0.50
1:AAA:69:ARG:HH22	4:AAA:206:PEG:H12	1.77	0.49
1:AAA:44[A]:GLN:HE21	6:AAA:205:DMS:C1	2.26	0.48
1:BBB:59:VAL:HG21	5:BBB:202:4NC:C4	2.43	0.48
1:BBB:98:GLU:CD	8:BBB:312:HOH:O	2.52	0.48
1:BBB:118[A]:GLN:HG2	8:BBB:374:HOH:O	2.14	0.47
1:AAA:85[A]:GLN:CD	8:AAA:305:HOH:O	2.53	0.47
1:AAA:55[B]:HIS:O	1:AAA:59:VAL:HG23	2.15	0.46
1:AAA:44[A]:GLN:HG2	6:AAA:205:DMS:C1	2.45	0.46
1:BBB:35:PHE:CE1	5:BBB:202:4NC:C6	2.99	0.46
1:BBB:59:VAL:HG21	5:BBB:202:4NC:C5	2.47	0.45
1:BBB:13:LEU:CD2	1:BBB:57[A]:GLU:HG3	2.46	0.45
4:AAA:203[B]:PEG:H22	4:AAA:203[B]:PEG:H41	1.45	0.45
1:AAA:10[B]:ARG:NH1	8:AAA:302:HOH:O	2.28	0.44
1:AAA:7:ALA:HA	4:AAA:203[A]:PEG:H42	1.99	0.44
1:AAA:59:VAL:HG21	5:AAA:204:4NC:C4	2.47	0.44
1:BBB:106:GLU:HG3	8:BBB:351:HOH:O	2.18	0.44
1:AAA:98[A]:GLU:CG	1:AAA:128:VAL:HG21	2.47	0.44
1:AAA:118[A]:GLN:HG2	3:AAA:207:GOL:O1	2.17	0.43
1:AAA:98[A]:GLU:HG3	1:AAA:128:VAL:HG21	2.01	0.43
1:AAA:43:ASP:HB2	6:AAA:205:DMS:H11	1.99	0.43
4:AAA:203[A]:PEG:O4	4:AAA:203[A]:PEG:H22	2.18	0.43
1:AAA:57[B]:GLU:O	1:AAA:57[B]:GLU:HG2	2.19	0.42
1:BBB:98:GLU:CG	1:BBB:128:VAL:HG21	2.48	0.42
1:BBB:48[B]:SER:HB3	8:BBB:304:HOH:O	2.20	0.42
1:AAA:43:ASP:HB2	6:AAA:205:DMS:C1	2.50	0.42
1:AAA:44[A]:GLN:HG2	6:AAA:205:DMS:H11	2.02	0.41
1:AAA:59:VAL:HG22	2:AAA:201:HEM:C4A	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:14[A]:ARG:CZ	1:AAA:57[A]:GLU:OE1	2.69	0.41
1:AAA:69:ARG:HH12	4:AAA:206:PEG:H11	1.84	0.41
1:BBB:118[A]:GLN:HG2	1:BBB:118[A]:GLN:H	1.67	0.41
1:AAA:122[B]:ARG:CZ	1:BBB:72[B]:ASP:OD2	2.70	0.40
1:BBB:21:PHE:CZ	5:BBB:202:4NC:C3	3.04	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	AAA	163/137 (119%)	159 (98%)	4 (2%)	0	100	100
1	BBB	160/137 (117%)	158 (99%)	1 (1%)	1 (1%)	25	7
All	All	323/274 (118%)	317 (98%)	5 (2%)	1 (0%)	34	18

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	37	ASN

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	AAA	145/117 (124%)	138 (95%)	7 (5%)	25 4
1	BBB	142/117 (121%)	138 (97%)	4 (3%)	43 11
All	All	287/234 (123%)	276 (96%)	11 (4%)	46 6

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	33[A]	ARG
1	AAA	33[B]	ARG
1	AAA	36	LYS
1	AAA	37[A]	ASN
1	AAA	37[B]	ASN
1	AAA	118[A]	GLN
1	AAA	118[B]	GLN
1	BBB	30[A]	ASP
1	BBB	30[B]	ASP
1	BBB	47[A]	LYS
1	BBB	47[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 ligands 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	$\# Z > 2$
3	GOL	AAA	207	-	5,5,5	0.20	0	5,5,5	0.26	0
4	PEG	AAA	203[B]	-	6,6,6	0.15	0	5,5,5	0.21	0
5	4NC	AAA	204	1	10,11,11	0.31	0	13,15,15	0.69	0
3	GOL	AAA	202	-	5,5,5	0.25	0	5,5,5	0.87	0
6	DMS	AAA	205	-	3,3,3	0.18	0	3,3,3	0.28	0
2	HEM	AAA	201	8,1	41,50,50	1.46	5 (12%)	45,82,82	1.78	11 (24%)
4	PEG	AAA	203[A]	-	6,6,6	0.44	0	5,5,5	0.38	0
7	SO4	BBB	203	-	4,4,4	0.54	0	6,6,6	0.66	0
2	HEM	BBB	201	8,1	41,50,50	1.47	10 (24%)	45,82,82	1.95	14 (31%)
5	4NC	BBB	202	1	10,11,11	0.34	0	13,15,15	0.79	0
4	PEG	AAA	206	-	6,6,6	0.69	0	5,5,5	0.62	0
7	SO4	BBB	204	-	4,4,4	0.69	0	6,6,6	0.25	0
7	SO4	AAA	208	-	4,4,4	0.22	0	6,6,6	0.14	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
3	GOL	AAA	207	-	-	2/4/4/4	-
4	PEG	AAA	203[B]	-	-	2/4/4/4	-
5	4NC	AAA	204	1	-	0/2/4/4	0/1/1/1
3	GOL	AAA	202	-	-	2/4/4/4	-
2	HEM	AAA	201	8,1	-	0/12/54/54	-
4	PEG	AAA	203[A]	-	-	3/4/4/4	-
2	HEM	BBB	201	8,1	-	4/12/54/54	-
5	4NC	BBB	202	1	-	0/2/4/4	0/1/1/1
4	PEG	AAA	206	-	-	4/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	201	HEM	C1B-NB	-3.56	1.34	1.40
2	AAA	201	HEM	C4B-NB	-3.08	1.32	1.38
2	BBB	201	HEM	C1B-NB	-2.84	1.35	1.40
2	AAA	201	HEM	FE-NB	2.74	2.10	1.96
2	BBB	201	HEM	C4D-C3D	2.66	1.49	1.45
2	AAA	201	HEM	C4D-C3D	2.51	1.49	1.45
2	AAA	201	HEM	C4D-ND	-2.46	1.36	1.40
2	BBB	201	HEM	C4B-NB	-2.46	1.33	1.38
2	BBB	201	HEM	FE-NB	2.41	2.08	1.96
2	BBB	201	HEM	CHB-C1B	2.33	1.40	1.35
2	BBB	201	HEM	C3C-C2C	2.27	1.43	1.40
2	BBB	201	HEM	C1D-C2D	2.19	1.48	1.44
2	BBB	201	HEM	C3B-C2B	-2.12	1.33	1.37
2	BBB	201	HEM	CBD-CAD	-2.10	1.45	1.52
2	BBB	201	HEM	C1A-NA	2.10	1.40	1.36

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	201	HEM	C4B-CHC-C1C	4.92	129.05	122.56
2	AAA	201	HEM	C1B-NB-C4B	4.77	110.00	105.07
2	BBB	201	HEM	C1B-NB-C4B	4.60	109.82	105.07
2	BBB	201	HEM	C4B-C3B-C2B	3.80	110.13	107.11
2	AAA	201	HEM	CHC-C4B-NB	3.56	128.30	124.43
2	BBB	201	HEM	C2C-C3C-C4C	-3.45	104.49	106.90
2	BBB	201	HEM	C3B-C2B-C1B	-3.22	104.10	106.49
2	BBB	201	HEM	CMC-C2C-C3C	3.17	130.61	124.68
2	AAA	201	HEM	CHB-C1B-NB	3.06	128.16	124.38
2	AAA	201	HEM	CAD-C3D-C4D	3.05	129.99	124.66
2	AAA	201	HEM	O2D-CGD-O1D	-2.95	115.96	123.30
2	BBB	201	HEM	CAD-CBD-CGD	-2.82	107.54	113.60
2	BBB	201	HEM	CHD-C1D-C2D	-2.70	120.75	124.98
2	AAA	201	HEM	C3D-C4D-ND	2.70	113.17	110.17
2	AAA	201	HEM	CHD-C1D-C2D	-2.65	120.84	124.98
2	BBB	201	HEM	CBA-CAA-C2A	-2.63	108.14	112.62
2	AAA	201	HEM	O2A-CGA-CBA	2.49	122.03	114.03
2	BBB	201	HEM	C1D-C2D-C3D	-2.48	104.35	106.96
2	BBB	201	HEM	C4A-C3A-C2A	-2.41	105.32	107.00
2	BBB	201	HEM	C2D-C1D-ND	2.37	112.73	109.88
2	AAA	201	HEM	CHD-C1D-ND	2.36	127.00	124.43
2	AAA	201	HEM	CHA-C4D-C3D	-2.13	121.32	125.33
2	AAA	201	HEM	O1A-CGA-CBA	-2.12	116.28	123.08
2	BBB	201	HEM	CHC-C4B-NB	2.07	126.68	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	201	HEM	CHB-C1B-NB	2.03	126.89	124.38

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	207	GOL	O1-C1-C2-O2
3	AAA	207	GOL	O1-C1-C2-C3
4	AAA	203[B]	PEG	C4-C3-O2-C2
4	AAA	203[A]	PEG	C4-C3-O2-C2
4	AAA	203[A]	PEG	O1-C1-C2-O2
4	AAA	206	PEG	C1-C2-O2-C3
2	BBB	201	HEM	C4D-C3D-CAD-CBD
4	AAA	203[B]	PEG	O2-C3-C4-O4
4	AAA	206	PEG	O2-C3-C4-O4
3	AAA	202	GOL	O1-C1-C2-C3
3	AAA	202	GOL	O1-C1-C2-O2
4	AAA	203[A]	PEG	O2-C3-C4-O4
4	AAA	206	PEG	O1-C1-C2-O2
4	AAA	206	PEG	C4-C3-O2-C2
2	BBB	201	HEM	CAD-CBD-CGD-O1D
2	BBB	201	HEM	C2D-C3D-CAD-CBD
2	BBB	201	HEM	CAD-CBD-CGD-O2D

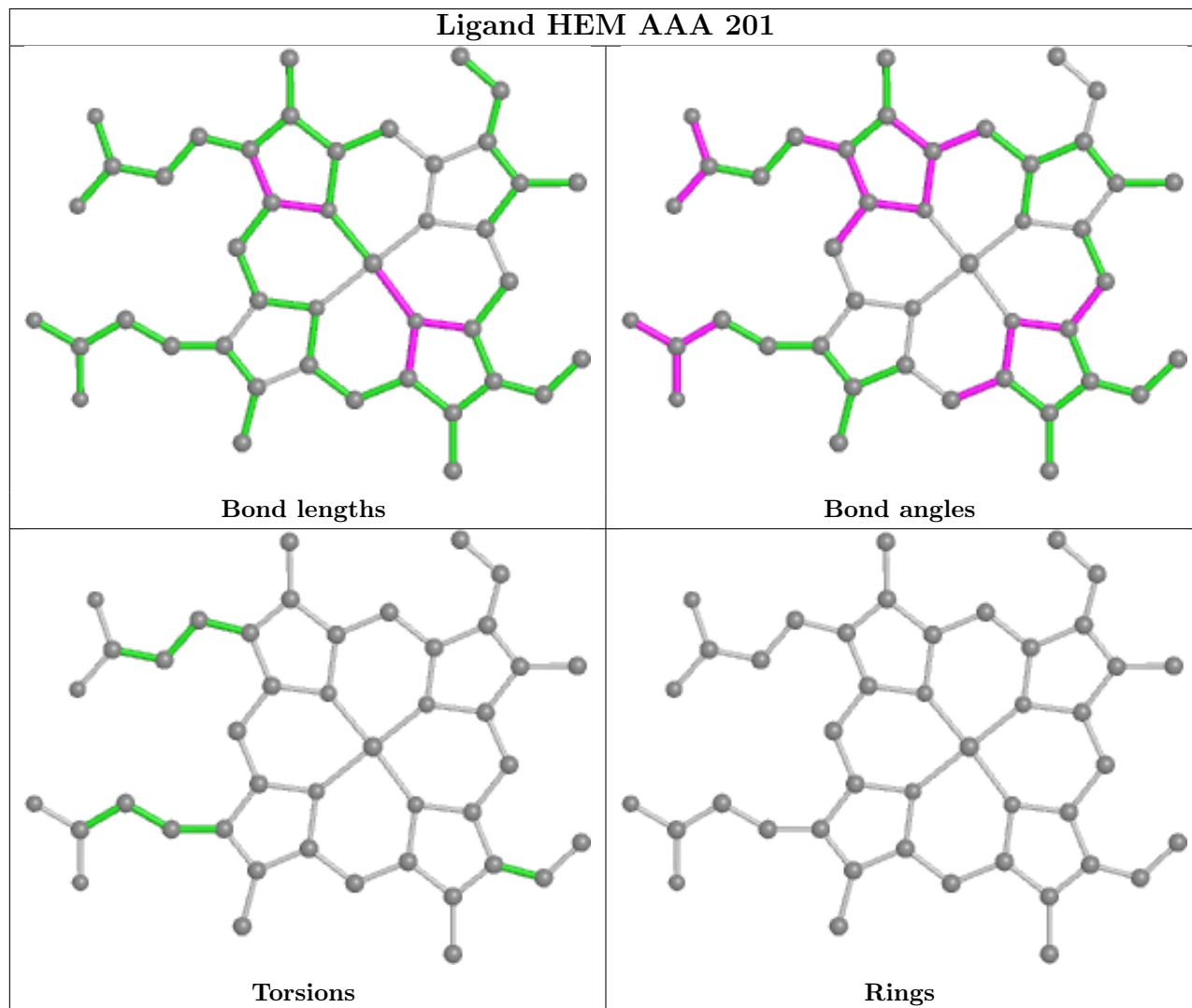
There are no ring outliers.

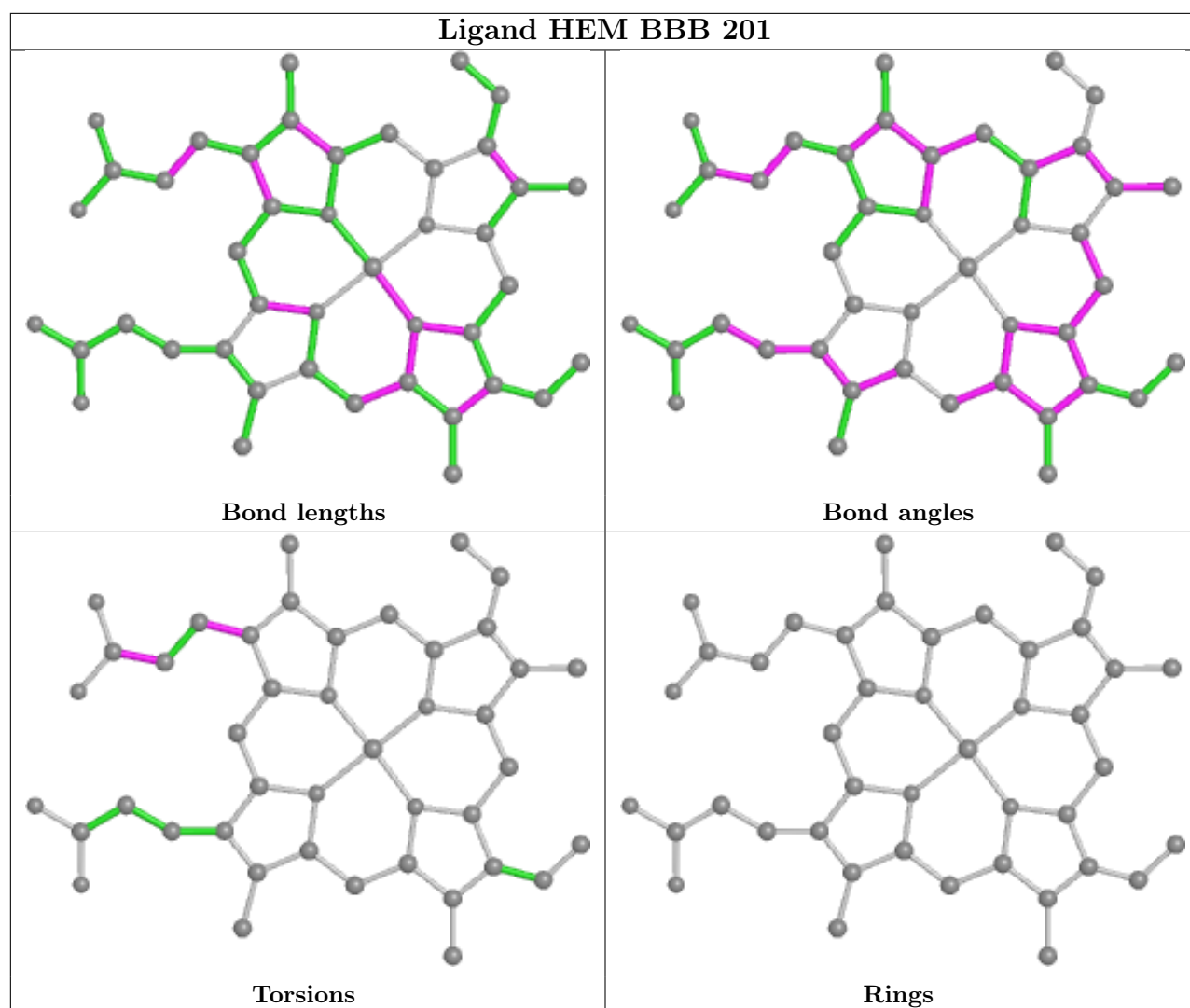
8 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	207	GOL	3	0
4	AAA	203[B]	PEG	1	0
5	AAA	204	4NC	5	0
6	AAA	205	DMS	5	0
2	AAA	201	HEM	3	0
4	AAA	203[A]	PEG	4	0
5	BBB	202	4NC	7	0
4	AAA	206	PEG	10	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	AAA	137/137 (100%)	0.04	2 (1%) 73 72	8, 15, 30, 42	0
1	BBB	137/137 (100%)	-0.25	2 (1%) 73 72	8, 12, 26, 37	0
All	All	274/274 (100%)	-0.10	4 (1%) 73 72	8, 13, 29, 42	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	91	SER	3.0
1	BBB	118[A]	GLN	2.3
1	AAA	50	ALA	2.2
1	BBB	36	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

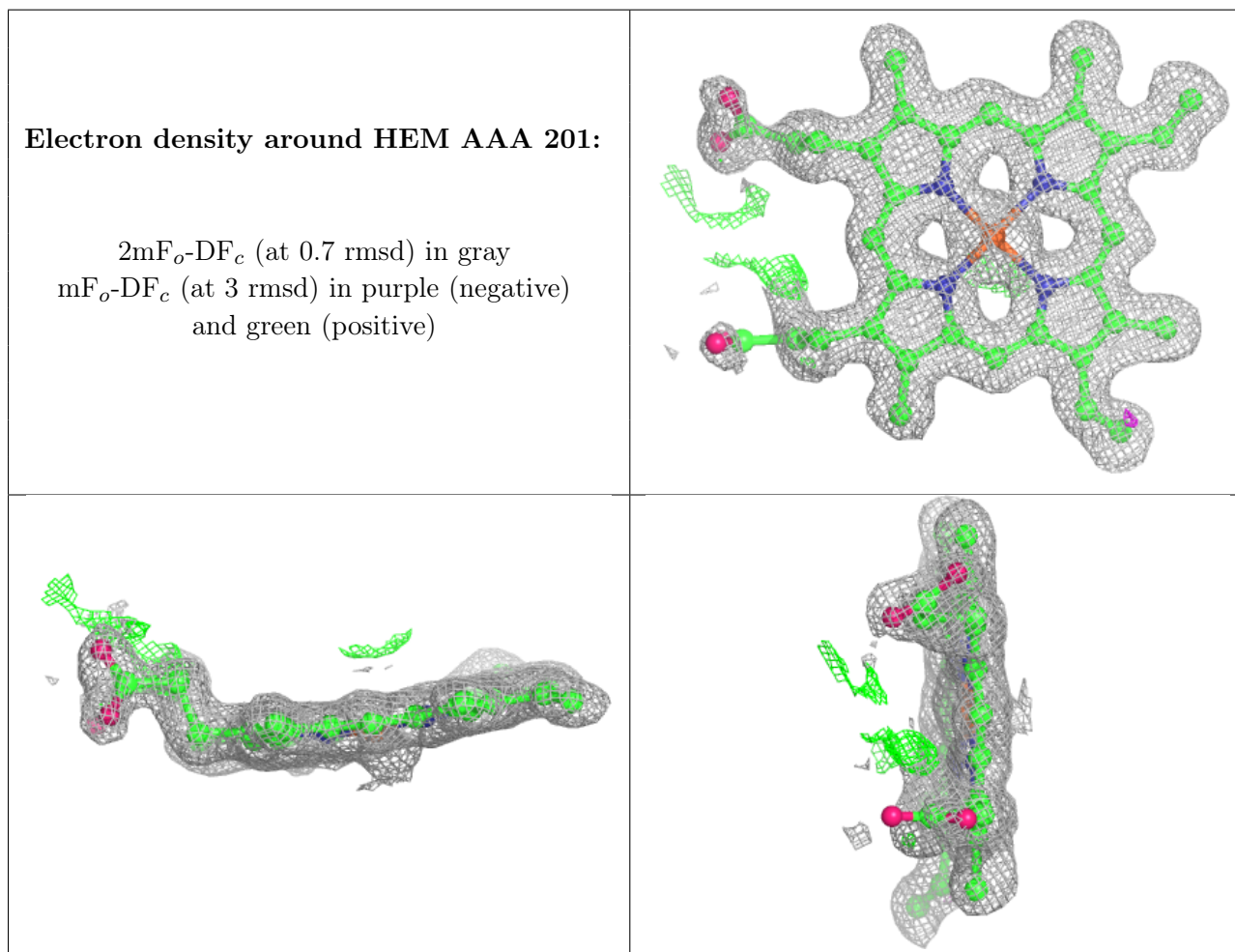
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PEG	AAA	206	7/7	0.80	0.31	22,25,33,35	0

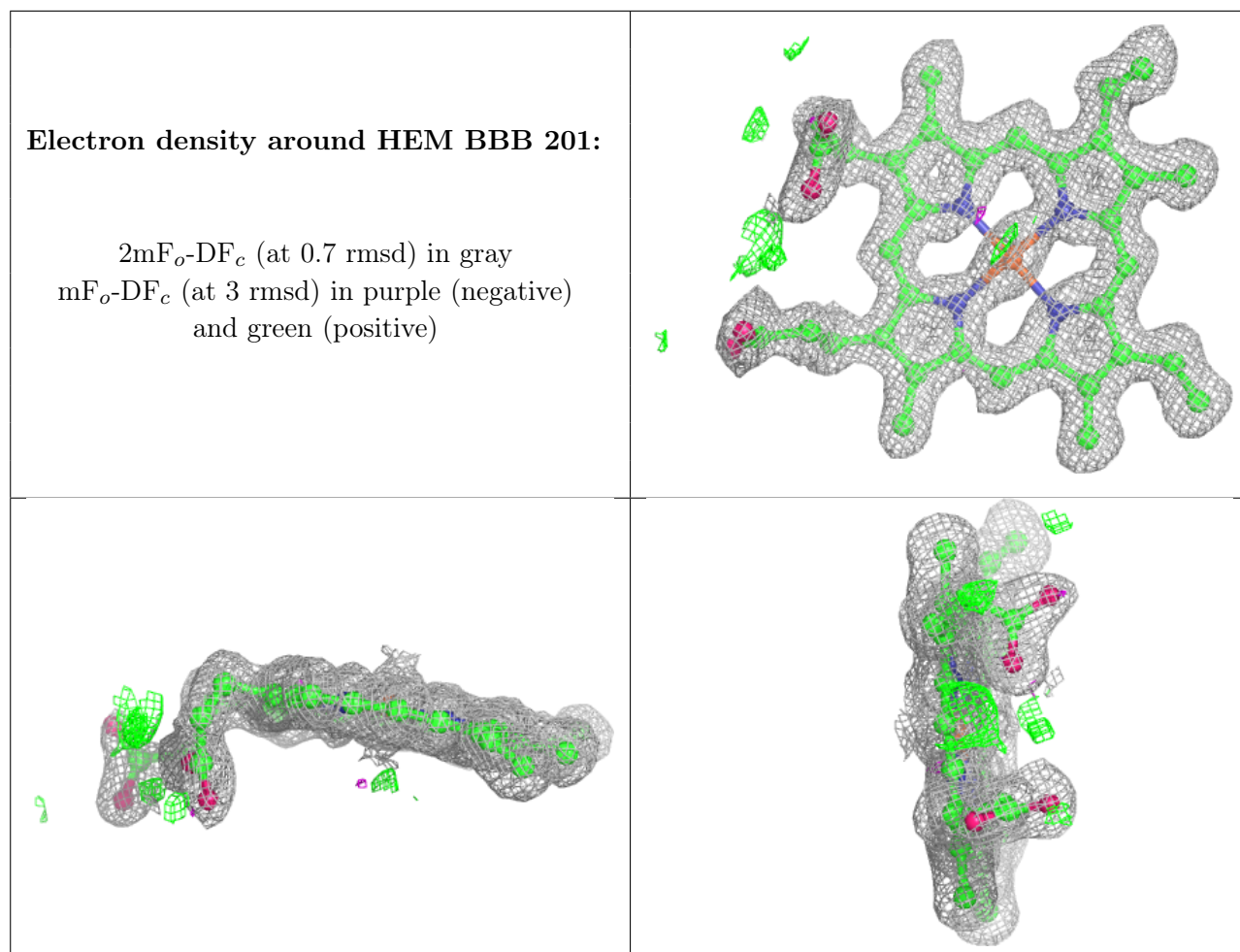
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	4NC	AAA	204	11/11	0.81	0.24	17,19,22,23	11
5	4NC	BBB	202	11/11	0.84	0.18	12,14,18,18	11
3	GOL	AAA	202	6/6	0.85	0.19	12,25,35,48	0
7	SO4	AAA	208	5/5	0.85	0.26	43,47,54,60	5
3	GOL	AAA	207	6/6	0.88	0.21	27,35,43,45	0
6	DMS	AAA	205	4/4	0.91	0.22	41,50,55,55	0
4	PEG	AAA	203[B]	7/7	0.92	0.27	11,17,31,37	7
4	PEG	AAA	203[A]	7/7	0.92	0.27	15,19,21,22	7
7	SO4	BBB	204	5/5	0.97	0.08	13,14,16,17	0
2	HEM	AAA	201	43/43	0.98	0.07	10,16,33,56	6
2	HEM	BBB	201	43/43	0.99	0.07	7,11,22,31	3
7	SO4	BBB	203	5/5	1.00	0.04	9,10,12,12	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.