



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:00 AM UTC

PDB ID : 8VKC / pdb_00008vkc
Title : Crystal structure of dehaloperoxidase A in complex with substrate 4-nitrophenol
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Deposited on : 2024-01-08
Resolution : 2.03 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

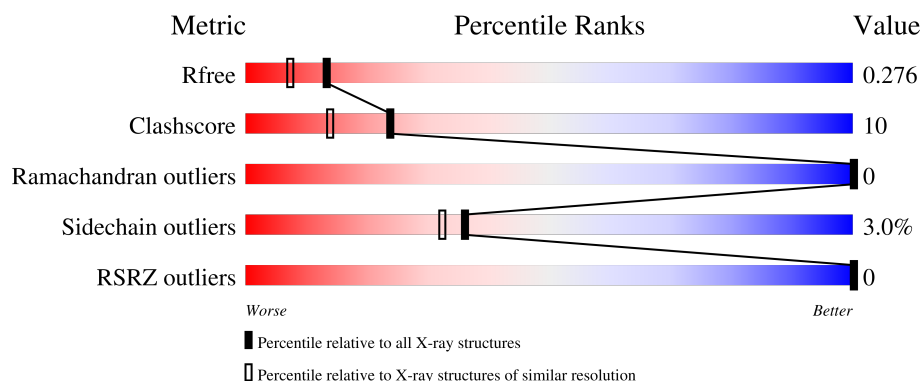
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	 83% 16% .
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
3	NPO	AAA	202	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2605 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.

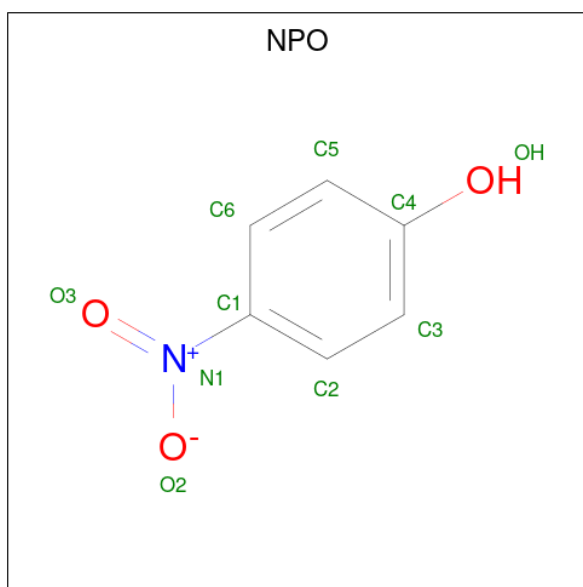
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	137	Total	C	N	O	S	0	13	0
			1193	746	210	229	8			
1	BBB	137	Total	C	N	O	S	0	13	0
			1182	740	207	227	8			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 P-NITROPHENOL (CCD ID: NPO) (formula: $C_6H_5NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	N	O	0	0
			10	6	1	3		
3	BBB	1	Total	C	N	O	0	0
			10	6	1	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	48	Total	O	0	0
			48	48		
6	BBB	55	Total	O	0	0
			55	55		

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:  83% 16% .



- 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	58.82Å 67.94Å 68.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.43 – 2.03 30.43 – 2.03	Depositor EDS
% Data completeness (in resolution range)	93.0 (30.43-2.03) 93.0 (30.43-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.154 , 0.275 0.164 , 0.276	Depositor DCC
R_{free} test set	841 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.035 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2605	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.69% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NPO, 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	1.05	1/1219 (0.1%)	1.43	2/1630 (0.1%)
1	BBB	1.07	0/1214	1.42	1/1624 (0.1%)
All	All	1.06	1/2433 (0.0%)	1.42	3/3254 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	74	VAL	N-CA	5.08	1.50	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	32	ARG	CA-C-N	5.07	127.39	120.54
1	AAA	32	ARG	C-N-CA	5.07	127.39	120.54
1	BBB	101	PHE	CA-CB-CG	-5.04	108.76	113.80

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	AAA	1193	0	1169	27	0
1	BBB	1182	0	1163	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AAA	43	0	30	6	0
2	BBB	43	0	30	2	0
3	AAA	10	0	4	4	0
3	BBB	10	0	5	2	0
4	AAA	6	0	8	0	0
5	BBB	15	0	0	1	0
6	AAA	48	0	0	2	0
6	BBB	55	0	0	3	0
All	All	2605	0	2409	50	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 10.

All (50) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:83:LEU:HA	1:AAA:86[A]:MET:HE2	1.66	0.78
1:AAA:94:THR:HG22	1:AAA:136:MET:CE	2.20	0.71
1:AAA:83:LEU:HA	1:AAA:86[A]:MET:CE	2.20	0.71
1:BBB:29:PRO:O	1:BBB:32[B]:ARG:HG3	1.93	0.68
1:AAA:55:HIS:HB3	3:AAA:202:NPO:OH	1.94	0.68
1:AAA:94:THR:CG2	1:AAA:136:MET:HE3	2.24	0.68
1:AAA:10[B]:ARG:HD3	6:AAA:305:HOH:O	1.96	0.65
1:AAA:94:THR:HB	1:AAA:128:VAL:HG13	1.81	0.63
2:AAA:201:HEM:HBB2	2:AAA:201:HEM:HMB2	1.83	0.61
1:AAA:83:LEU:HD23	1:AAA:86[A]:MET:HE1	1.83	0.60
1:BBB:131:LEU:HB3	1:BBB:136[A]:MET:HE2	1.85	0.59
1:AAA:82:THR:O	1:AAA:86[B]:MET:HG3	2.04	0.58
1:BBB:32[B]:ARG:HG3	1:BBB:32[B]:ARG:HH11	1.68	0.58
1:AAA:131:LEU:HB3	1:AAA:136:MET:HE2	1.86	0.57
1:BBB:36:LYS:HE2	1:BBB:37[B]:ASN:HB2	1.87	0.56
1:AAA:59:VAL:HG13	2:AAA:201:HEM:C1B	2.41	0.55
1:AAA:56:THR:HG22	3:AAA:202:NPO:H5	1.91	0.53
1:AAA:13[A]:LEU:HD23	1:AAA:13[A]:LEU:O	2.09	0.52
2:AAA:201:HEM:HMC1	2:AAA:201:HEM:HBC2	1.92	0.51
1:AAA:21:PHE:CD1	3:AAA:202:NPO:H6	2.46	0.51
1:BBB:52:PHE:O	1:BBB:56:THR:HG23	2.12	0.50
1:AAA:21:PHE:CE1	3:AAA:202:NPO:C6	2.95	0.49
1:BBB:37[A]:ASN:HD22	1:BBB:37[A]:ASN:N	2.10	0.49
2:AAA:201:HEM:HBB2	2:AAA:201:HEM:CMB	2.42	0.48
1:BBB:32[B]:ARG:NH2	5:BBB:203:SO4:S	2.86	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:55:HIS:HB3	3:BBB:202:NPO:OH	2.13	0.48
1:BBB:94:THR:N	1:BBB:136[A]:MET:HE3	2.29	0.47
1:BBB:99:LYS:NZ	6:BBB:304:HOH:O	2.43	0.47
2:BBB:201:HEM:HMC1	2:BBB:201:HEM:HBC2	1.95	0.47
1:AAA:14[A]:ARG:NH1	1:AAA:53:GLY:HA3	2.30	0.47
1:AAA:83:LEU:HD23	1:AAA:86[A]:MET:CE	2.45	0.47
2:AAA:201:HEM:HBC2	2:AAA:201:HEM:CMC	2.46	0.45
1:AAA:105:VAL:O	1:AAA:109[A]:ARG:HG3	2.16	0.45
1:BBB:87:LYS:HG2	6:BBB:333:HOH:O	2.16	0.45
1:BBB:59:VAL:HG21	3:BBB:202:NPO:C2	2.47	0.45
1:AAA:94:THR:CG2	1:AAA:136:MET:CE	2.85	0.44
1:AAA:94:THR:HG23	1:AAA:136:MET:HE3	1.97	0.43
1:BBB:132[B]:SER:HB2	6:BBB:303:HOH:O	2.19	0.43
1:AAA:55:HIS:HD2	2:AAA:201:HEM:O1D	2.02	0.43
2:BBB:201:HEM:HMB2	2:BBB:201:HEM:HBB2	2.01	0.42
1:AAA:44:GLN:HB2	6:AAA:319:HOH:O	2.19	0.42
1:BBB:94:THR:HB	1:BBB:128:VAL:HG13	2.02	0.42
1:AAA:13[A]:LEU:HD23	1:AAA:13[A]:LEU:C	2.44	0.42
1:BBB:94:THR:CA	1:BBB:136[A]:MET:HE3	2.50	0.42
1:AAA:122[A]:ARG:HE	1:BBB:72:ASP:CG	2.28	0.41
1:AAA:14[A]:ARG:NH2	1:AAA:54:ASP:OD1	2.38	0.41
1:AAA:94:THR:HA	1:AAA:136:MET:CE	2.50	0.41
1:BBB:37[A]:ASN:ND2	1:BBB:37[A]:ASN:H	2.19	0.41
1:AAA:94:THR:CA	1:AAA:136:MET:HE3	2.51	0.40
1:BBB:36:LYS:HG2	1:BBB:37[A]:ASN:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	148/137 (108%)	145 (98%)	3 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BBB	148/137 (108%)	146 (99%)	2 (1%)	0	100	100
All	All	296/274 (108%)	291 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	AAA	130/117 (111%)	128 (98%)	2 (2%)	57	59
1	BBB	130/117 (111%)	124 (95%)	6 (5%)	24	17
All	All	260/234 (111%)	252 (97%)	8 (3%)	36	31

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	44	GLN
1	AAA	137	LYS
1	BBB	36	LYS
1	BBB	37[A]	ASN
1	BBB	37[B]	ASN
1	BBB	48	SER
1	BBB	98	GLU
1	BBB	118	GLN

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

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
5	SO4	BBB	204	-	4,4,4	0.32	0	6,6,6	0.14	0
5	SO4	BBB	205	-	4,4,4	0.30	0	6,6,6	0.08	0
3	NPO	BBB	202	-	10,10,10	0.71	0	11,13,13	0.88	0
4	GOL	AAA	203	-	5,5,5	0.06	0	5,5,5	0.33	0
5	SO4	BBB	203	-	4,4,4	0.33	0	6,6,6	0.14	0
2	HEM	BBB	201	1	50,50,50	1.70	10 (20%)	67,82,82	1.60	13 (19%)
3	NPO	AAA	202	-	10,10,10	0.64	0	11,13,13	0.77	0
2	HEM	AAA	201	1	50,50,50	1.55	6 (12%)	67,82,82	1.58	12 (17%)

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	NPO	BBB	202	-	-	1/2/4/4	0/1/1/1
4	GOL	AAA	203	-	-	3/4/4/4	-
2	HEM	BBB	201	1	-	2/14/54/54	-
3	NPO	AAA	202	-	-	0/2/4/4	0/1/1/1
2	HEM	AAA	201	1	-	2/14/54/54	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	201	HEM	FE-NB	4.80	2.09	1.94
2	BBB	201	HEM	FE-NB	4.68	2.09	1.94
2	AAA	201	HEM	FE-NC	4.45	2.09	1.95
2	BBB	201	HEM	FE-NC	4.10	2.08	1.95
2	AAA	201	HEM	C4D-ND	-3.49	1.34	1.40
2	BBB	201	HEM	C4D-ND	-3.45	1.34	1.40
2	AAA	201	HEM	C1B-NB	-3.41	1.34	1.40
2	BBB	201	HEM	C3C-C4C	-3.24	1.40	1.46
2	BBB	201	HEM	C4B-NB	-3.18	1.32	1.38
2	BBB	201	HEM	C4D-C3D	3.08	1.50	1.45
2	BBB	201	HEM	C1C-C2C	-2.66	1.40	1.45
2	BBB	201	HEM	C1B-NB	-2.66	1.35	1.40
2	BBB	201	HEM	C4C-NC	-2.56	1.34	1.39
2	AAA	201	HEM	O2A-CGA	-2.45	1.22	1.30
2	AAA	201	HEM	C4B-NB	-2.17	1.34	1.38
2	BBB	201	HEM	C3B-C4B	2.03	1.48	1.44

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	201	HEM	CHC-C4B-NB	4.99	129.79	124.42
2	BBB	201	HEM	CHC-C4B-NB	4.85	129.64	124.42
2	AAA	201	HEM	CHD-C1D-ND	4.11	128.84	124.42
2	BBB	201	HEM	CHD-C1D-C2D	-4.03	118.66	125.03
2	AAA	201	HEM	C1B-NB-C4B	3.82	109.73	105.21
2	BBB	201	HEM	C2D-C1D-ND	3.41	113.84	109.90
2	AAA	201	HEM	CHA-C4D-ND	3.08	128.18	124.37
2	BBB	201	HEM	C1B-NB-C4B	2.84	108.56	105.21
2	BBB	201	HEM	CHD-C1D-ND	2.82	127.46	124.42
2	AAA	201	HEM	CHD-C1D-C2D	-2.81	120.60	125.03
2	BBB	201	HEM	C1D-C2D-C3D	-2.78	104.06	106.98
2	BBB	201	HEM	CHA-C4D-ND	2.73	127.74	124.37
2	AAA	201	HEM	CHA-C4D-C3D	-2.69	120.27	125.23
2	AAA	201	HEM	O2A-CGA-CBA	2.66	122.42	114.00
2	AAA	201	HEM	C4B-C3B-C2B	-2.66	104.84	107.28
2	BBB	201	HEM	C4A-C3A-C2A	2.58	109.77	106.82
2	AAA	201	HEM	CAD-C3D-C4D	2.57	129.18	124.70
2	BBB	201	HEM	O2D-CGD-CBD	2.54	122.01	114.00
2	BBB	201	HEM	CBA-CAA-C2A	-2.43	105.80	112.53
2	AAA	201	HEM	CHB-C1B-NB	2.32	127.23	124.37
2	AAA	201	HEM	CMD-C2D-C1D	2.25	128.55	125.03
2	AAA	201	HEM	O2A-CGA-O1A	-2.21	117.65	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	201	HEM	CHD-C4C-NC	2.21	126.86	124.45
2	BBB	201	HEM	O2A-CGA-CBA	2.13	120.73	114.00
2	BBB	201	HEM	CHC-C4B-C3B	-2.01	121.07	125.07

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	203	GOL	O1-C1-C2-C3
4	AAA	203	GOL	C1-C2-C3-O3
2	BBB	201	HEM	C4D-C3D-CAD-CBD
2	BBB	201	HEM	C2D-C3D-CAD-CBD
4	AAA	203	GOL	O2-C2-C3-O3
3	BBB	202	NPO	C2-C1-N1-O3
2	AAA	201	HEM	CAD-CBD-CGD-O2D
2	AAA	201	HEM	CAD-CBD-CGD-O1D

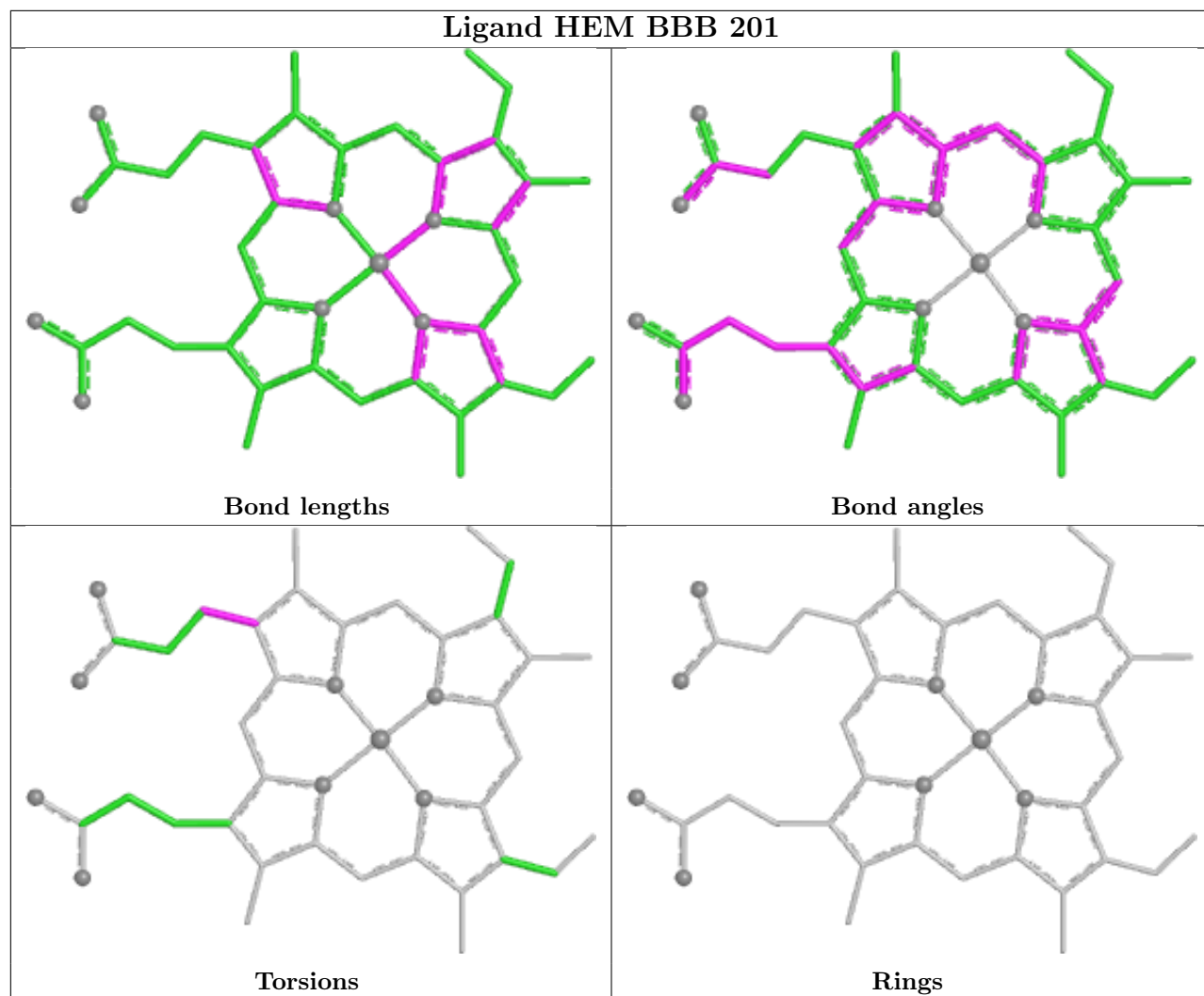
There are no ring outliers.

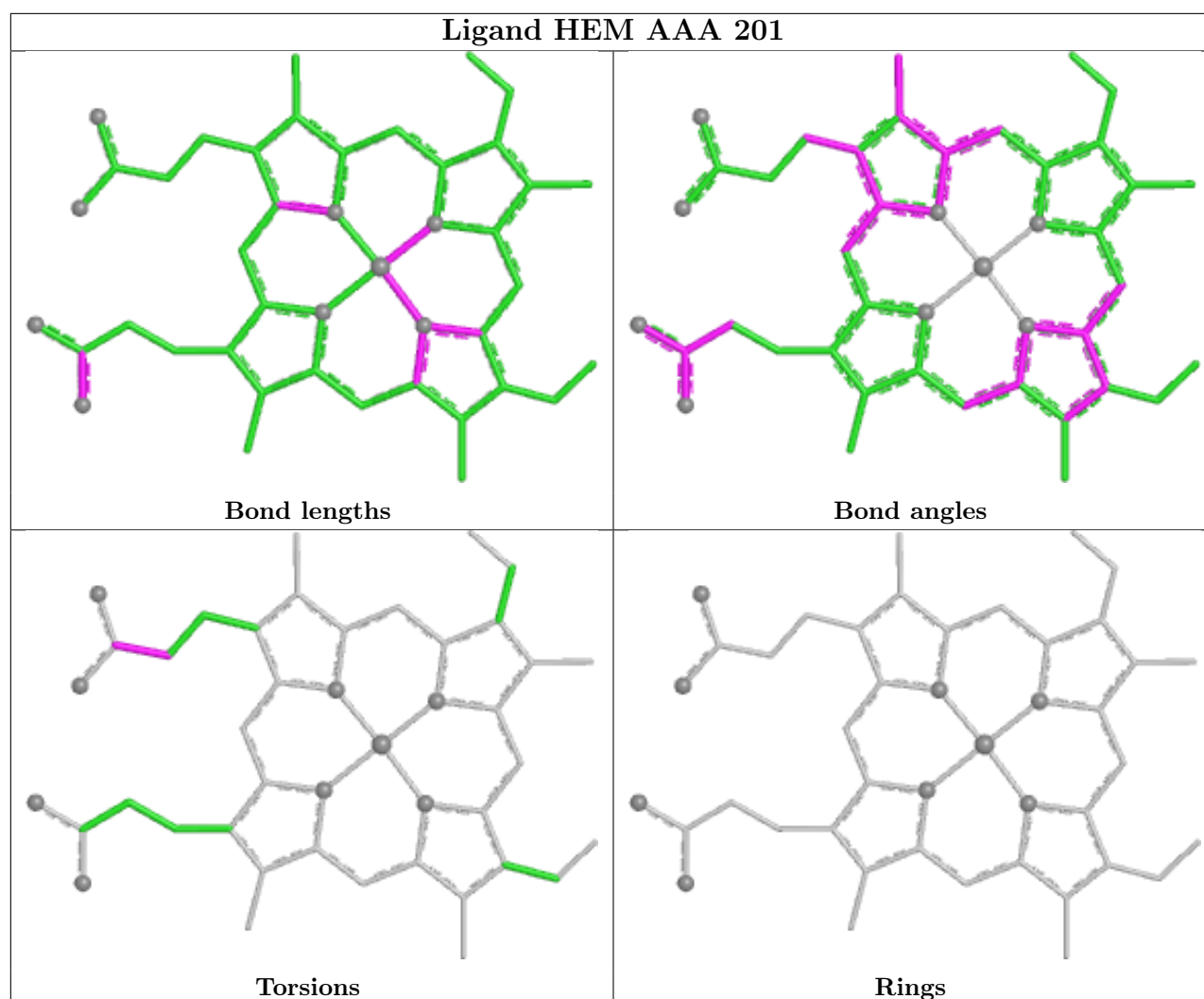
5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	BBB	202	NPO	2	0
5	BBB	203	SO4	1	0
2	BBB	201	HEM	2	0
3	AAA	202	NPO	4	0
2	AAA	201	HEM	6	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.

Ligand HEM BBB 201





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%)	-0.34	0 100 100	12, 29, 48, 64	13 (9%)
1	BBB	137/137 (100%)	-0.41	0 100 100	13, 26, 40, 66	13 (9%)
All	All	274/274 (100%)	-0.37	0 100 100	12, 27, 46, 66	26 (9%)

There are no RSRZ outliers to report.

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 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
3	NPO	AAA	202	10/10	0.81	0.15	31,32,36,42	10
3	NPO	BBB	202	10/10	0.87	0.10	33,40,46,48	0
5	SO4	BBB	205	5/5	0.94	0.07	69,72,73,76	0
4	GOL	AAA	203	6/6	0.95	0.08	35,41,43,47	0
2	HEM	AAA	201	43/43	0.97	0.07	24,31,50,61	6
5	SO4	BBB	204	5/5	0.98	0.05	32,33,36,40	0
2	HEM	BBB	201	43/43	0.98	0.06	20,24,32,65	3

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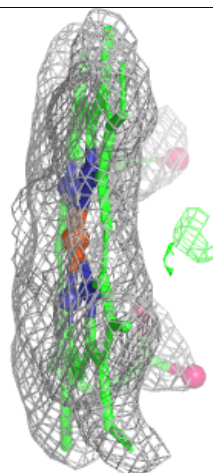
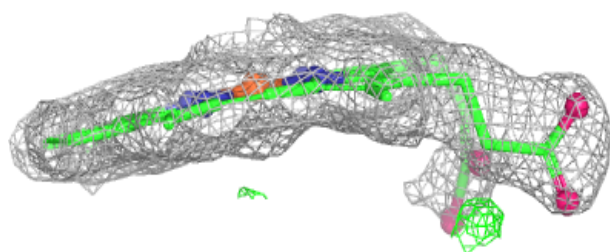
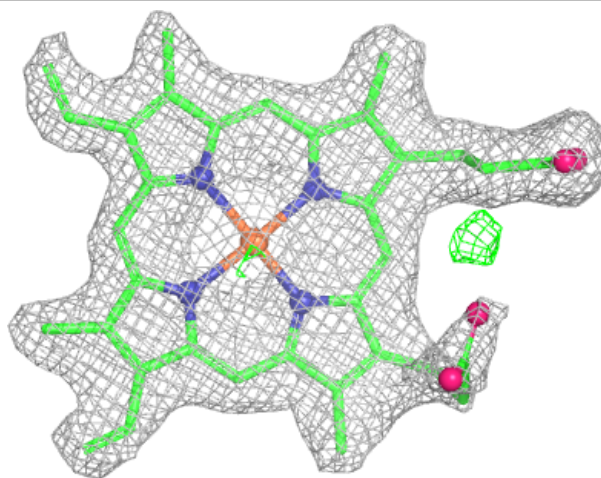
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	BBB	203	5/5	0.99	0.04	21,21,25,27	0

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.

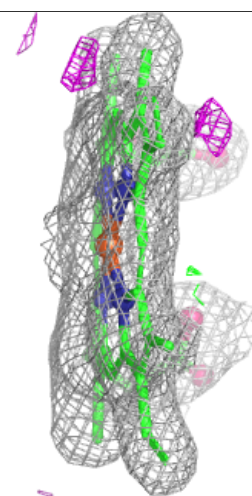
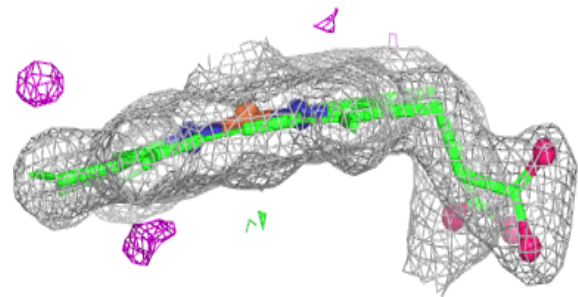
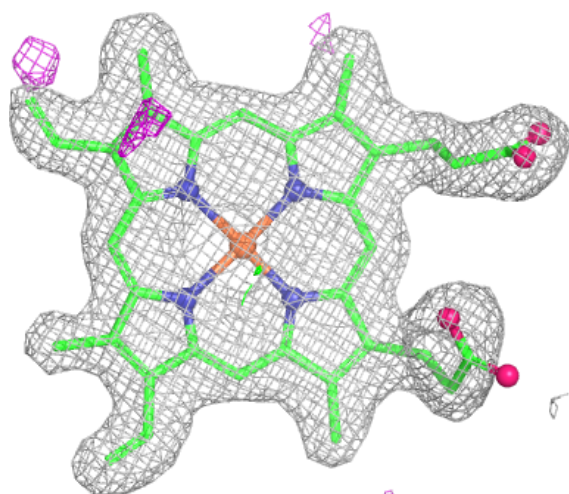
Electron density around HEM AAA 201:

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



Electron density around HEM BBB 201:

$2mF_o-DF_c$ (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.