



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 01:30 am BST

PDB ID : 5KSN
Title : Crystal structure of the S324G variant of catalase-peroxidase from *B. pseudo-mallei* with INH bound
Authors : Loewen, P.C.
Deposited on : 2016-07-08
Resolution : 1.87 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

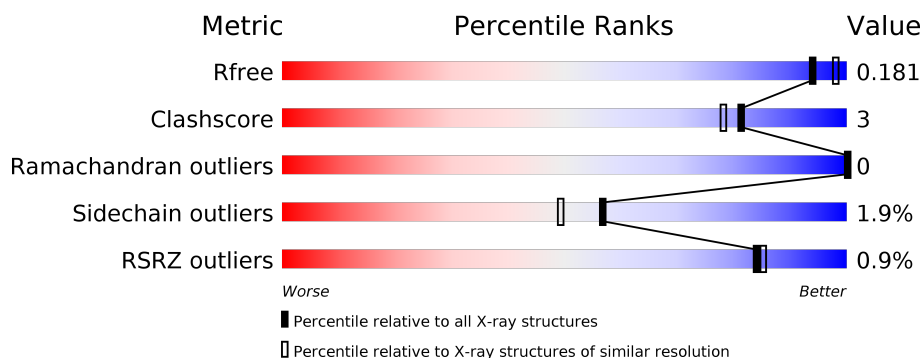
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 on 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	728	<div> <div></div> <div>87%</div> <div>9%</div> <div>..</div> </div>
1	B	728	<div> <div></div> <div>86%</div> <div>11%</div> <div>..</div> </div>

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
8	NIZ	A	809	-	X	-	-

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.

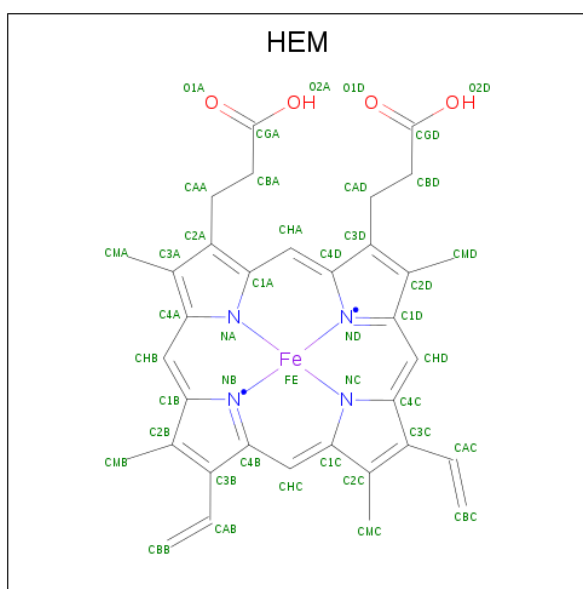
- Molecule 1 is a protein called Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total 5555	C 3508	N 989	O 1044	S 14	0	7	0
1	B	713	Total 5581	C 3523	N 994	O 1050	S 14	0	10	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	324	GLY	SER	engineered mutation	UNP Q3JNW6
B	324	GLY	SER	engineered mutation	UNP Q3JNW6

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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

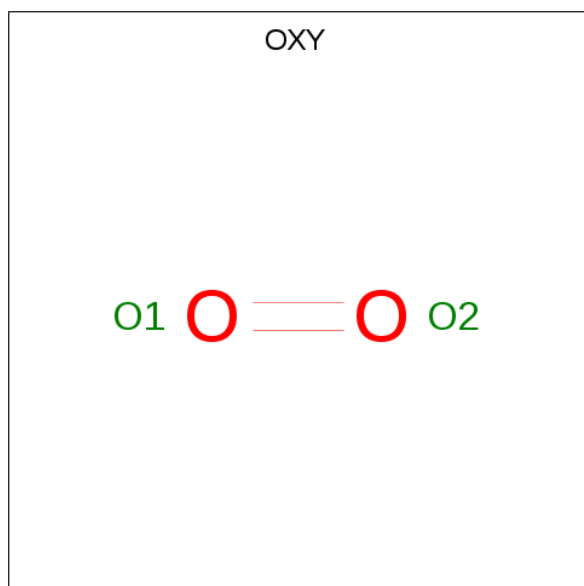
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na		
			1	1	0	0
3	A	1	Total	Na		
			1	1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O		
			2	2	0	0
5	A	1	Total	O		
			2	2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	O	0	0
			2	2		
5	B	1	Total	O	0	0
			2	2		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



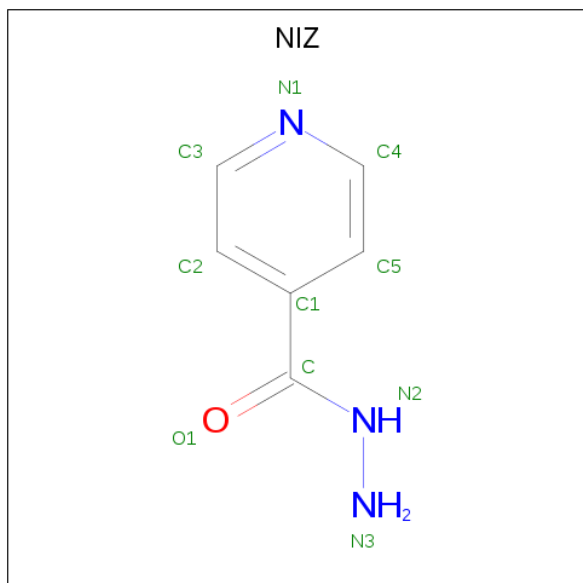
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			8	6	2		
7	A	1	Total	C	O	0	0
			8	6	2		
7	B	1	Total	C	O	0	0
			8	6	2		
7	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 8 is pyridine-4-carbohydrazide (three-letter code: NIZ) (formula: $C_6H_7N_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total 10	C 6	N 3	O 1	0	0
8	B	1	Total 10	C 6	N 3	O 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	786	Total 786	O 786	0	0
9	B	821	Total 821	O 821	0	0

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

Chain A:

Residue	Residue	Residue	Residue	Residue	Residue
Met	E584	Ser	E589	Asn	S590
Ser	R218	Ala	M591	Glu	A592
Ala	N247	Pro	R255	Lys	L594
Lys	R263	Phe	R263	Cys	R602
Cys	D268	His	E269	Pro	K608
Phe	E269	Gln	T284	Ala	Y609
His	T284	Ala	E277	Gly	R610
Gln	E277	Gly	E343	Asn	V611
Ala	E343	Asn	E349	Gln	Q622
Ala	E349	Gln	D376	Ala	V633
Gly	D376	Asn	K379	Glu	V645
Asn	K379	Glu	D395	Pro	G646
Gln	D395	Pro	R403	His	Q647
Gln	R403	His	R404	Gln	S648
Ala	R404	Gln	E407	Ala	R649
Ala	E407	Ala	R418	Gly	D670
Asn	R418	Gly	R426	Asn	A679
Asn	R426	Asn	D427	Gln	A680
Gln	D427	Gln	M428	Pro	R701
Gln	M428	Pro	R431	His	Q711
Pro	R431	His	A432	Gln	L712
His	A432	Gln	R433	Ala	R713
His	R433	Ala	Y434	Lys	Y719
Ala	Y434	Lys	E438	Pro	Q725
Ala	E438	Pro	D454	His	E726
Gly	D454	His	D459	Gln	R730
Gly	D459	Gln	R497	Ala	W736
Ala	R497	Ala	E529	Glu	A748
Glu	E529	Glu	R532	Pro	
Glu	R532	Pro	G541	His	
Pro	G541	His	O540	Ala	
His	O540	Ala		Glu	

Chain B:

86% 11%

Label	Color
E198	Green
D199	Green
R218	Green
Y238	Green
R255	Green
R258	Green
R263	Green
D268	Green
Y313	Green
E327	Green
D376	Green
K379	Green
R403	Green
H406	Green
E410	Green
F411	Green
F412	Green
A413	Green
D414	Green
R426	Green
D427	Green
M428	Green
R431	Green
A432	Green
R433	Green
Y434	Green
E438	Green
Q447	Green
D459	Green
R497	Green
R504	Green
I505	Green
R506	Green
D512	Green
W513	Green
E514	Green
E519	Green
E529	Green
R532	Green
R540	Green
G541	Green
Q544	Green
E560	Green
M591	Green
A592	Green
V593	Green
L594	Green
R602	Green
K608	Green
Y609	Green
R610	Green
Q622	Green
V633	Green
Q647	Green
S648	Green
R649	Green
T654	Green
E657	Green
N662	Green
A679	Green
A680	Green
D683	Green
E686	Green
G687	Green
R688	Green
D689	Green
R690	Green
K696	Green
H709	Green
S710	Green
Q711	Green
I712	Green
R713	Green
Y719	Green
Q725	Green
E726	Green
R730	Green
R744	Green
A748	Green
MET	Grey
SER	Grey
ASN	Grey
GLU	Grey
ALA	Grey
LYS	Grey
CYS	Grey
PRO	Grey
PHE	Grey
HIS	Grey
GLN	Grey
ALA	Grey
ALA	Grey
GLY	Grey
ASN	Grey
G36	Yellow
R40	Orange
Q46	Orange
L47	Orange
D48	Orange
R54	Orange
H55	Orange
G63	Orange
K64	Orange
D65	Orange
D76	Orange
R82	Orange
D83	Orange
R108	Orange
W111	Orange
R118	Orange
T119	Orange
R123	Orange
D141	Orange
N144	Orange
L145	Orange
D146	Orange
R149	Orange
R161	Orange
E178	Orange
K183	Orange
E196	Orange
P197	Orange

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.43Å 115.28Å 174.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.05 – 1.87 48.05 – 1.87	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.05-1.87) 98.6 (48.05-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.141 , 0.171 0.154 , 0.181	Depositor DCC
R_{free} test set	8235 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12903	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: MPD, OXY, CL, NA, PO4, NIZ, HEM

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	1.34	28/5706 (0.5%)	1.27	61/7757 (0.8%)
1	B	1.36	31/5735 (0.5%)	1.19	44/7795 (0.6%)
All	All	1.35	59/11441 (0.5%)	1.23	105/15552 (0.7%)

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	410	GLU	CG-CD	9.37	1.66	1.51
1	B	426	ARG	CZ-NH2	9.01	1.44	1.33
1	A	589	GLU	CD-OE2	8.09	1.34	1.25
1	B	438	GLU	CD-OE1	-7.85	1.17	1.25
1	B	434	TYR	CE1-CZ	-7.68	1.28	1.38

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	161	ARG	NE-CZ-NH1	19.12	129.86	120.30
1	A	255[A]	ARG	NE-CZ-NH2	-16.83	111.88	120.30
1	A	255[B]	ARG	NE-CZ-NH2	-16.83	111.88	120.30
1	A	255[A]	ARG	NE-CZ-NH1	11.63	126.11	120.30
1	A	255[B]	ARG	NE-CZ-NH1	11.63	126.11	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5555	0	5368	23	0
1	B	5581	0	5391	30	0
2	A	43	0	30	1	0
2	B	43	0	30	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	1	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	16	0	28	3	0
7	B	16	0	28	1	0
8	A	10	0	7	2	0
8	B	10	0	7	1	0
9	A	786	0	0	5	1
9	B	821	0	0	13	1
All	All	12903	0	10889	58	1

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 3.

The worst 5 of 58 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:A:725[A]:GLN:NE2	1:A:726[A]:GLU:HG3	1.45	1.30
1:A:622[A]:GLN:NE2	8:A:809:NIZ:O1	1.91	1.04
1:B:622[A]:GLN:NE2	8:B:809:NIZ:O1	1.96	0.97
1:A:725[A]:GLN:NE2	1:A:726[A]:GLU:CG	2.30	0.94
1:A:119[B]:THR:HG21	9:A:1114:HOH:O	1.74	0.87

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1251:HOH:O	9:B:1149:HOH:O[2_444]	2.01	0.19

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	A	718/728 (99%)	710 (99%)	8 (1%)	0	100	100
1	B	721/728 (99%)	711 (99%)	10 (1%)	0	100	100
All	All	1439/1456 (99%)	1421 (99%)	18 (1%)	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	A	556/560 (99%)	543 (98%)	13 (2%)	50	41
1	B	559/560 (100%)	548 (98%)	11 (2%)	55	47
All	All	1115/1120 (100%)	1091 (98%)	24 (2%)	57	43

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	649	ARG
1	B	40	ARG
1	B	649	ARG
1	A	725[A]	GLN
1	A	725[B]	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	227	ASN
1	B	725	GLN
1	B	544	GLN
1	A	520	GLN
1	B	520	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	OXY	B	804	-	1,1,1	0.19	0	-		
5	OXY	A	804	-	1,1,1	0.05	0	-		
7	MPD	B	807	-	7,7,7	0.52	0	9,10,10	1.48	1 (11%)
2	HEM	B	801	1,9	27,50,50	1.50	4 (14%)	17,82,82	2.18	6 (35%)
8	NIZ	A	809	-	10,10,10	2.86	4 (40%)	12,12,12	3.42	9 (75%)
6	PO4	A	806	-	4,4,4	1.78	1 (25%)	6,6,6	2.51	2 (33%)
5	OXY	B	805	-	1,1,1	0.23	0	-		
6	PO4	B	806	-	4,4,4	1.00	0	6,6,6	1.98	3 (50%)
5	OXY	A	805	-	1,1,1	0.31	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MPD	A	808	-	7,7,7	0.73	0	9,10,10	1.76	2 (22%)
7	MPD	A	807	-	7,7,7	0.54	0	9,10,10	1.12	0
8	NIZ	B	809	-	10,10,10	2.97	4 (40%)	12,12,12	3.15	7 (58%)
2	HEM	A	801	1,9	27,50,50	1.21	3 (11%)	17,82,82	1.96	7 (41%)
7	MPD	B	808	-	7,7,7	0.70	0	9,10,10	1.62	4 (44%)

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
7	MPD	B	807	-	-	3/5/5/5	-
2	HEM	B	801	1,9	-	0/6/54/54	-
8	NIZ	A	809	-	-	0/6/6/6	0/1/1/1
7	MPD	A	807	-	-	0/5/5/5	-
7	MPD	A	808	-	-	0/5/5/5	-
8	NIZ	B	809	-	-	0/6/6/6	0/1/1/1
2	HEM	A	801	1,9	-	0/6/54/54	-
7	MPD	B	808	-	-	3/5/5/5	-

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	809	NIZ	N3-N2	-7.07	1.31	1.41
8	B	809	NIZ	N3-N2	-6.34	1.32	1.41
2	B	801	HEM	C3B-C2B	-5.23	1.33	1.40
8	B	809	NIZ	C4-N1	4.26	1.46	1.33
8	B	809	NIZ	C5-C1	4.06	1.46	1.39

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	809	NIZ	O1-C-C1	-6.30	109.70	120.94
8	B	809	NIZ	C1-C-N2	5.73	122.82	116.27
2	B	801	HEM	CAA-CBA-CGA	-5.39	103.63	112.67
8	B	809	NIZ	C5-C4-N1	-5.31	114.38	123.62
6	A	806	PO4	O4-P-O3	5.23	124.75	107.97

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

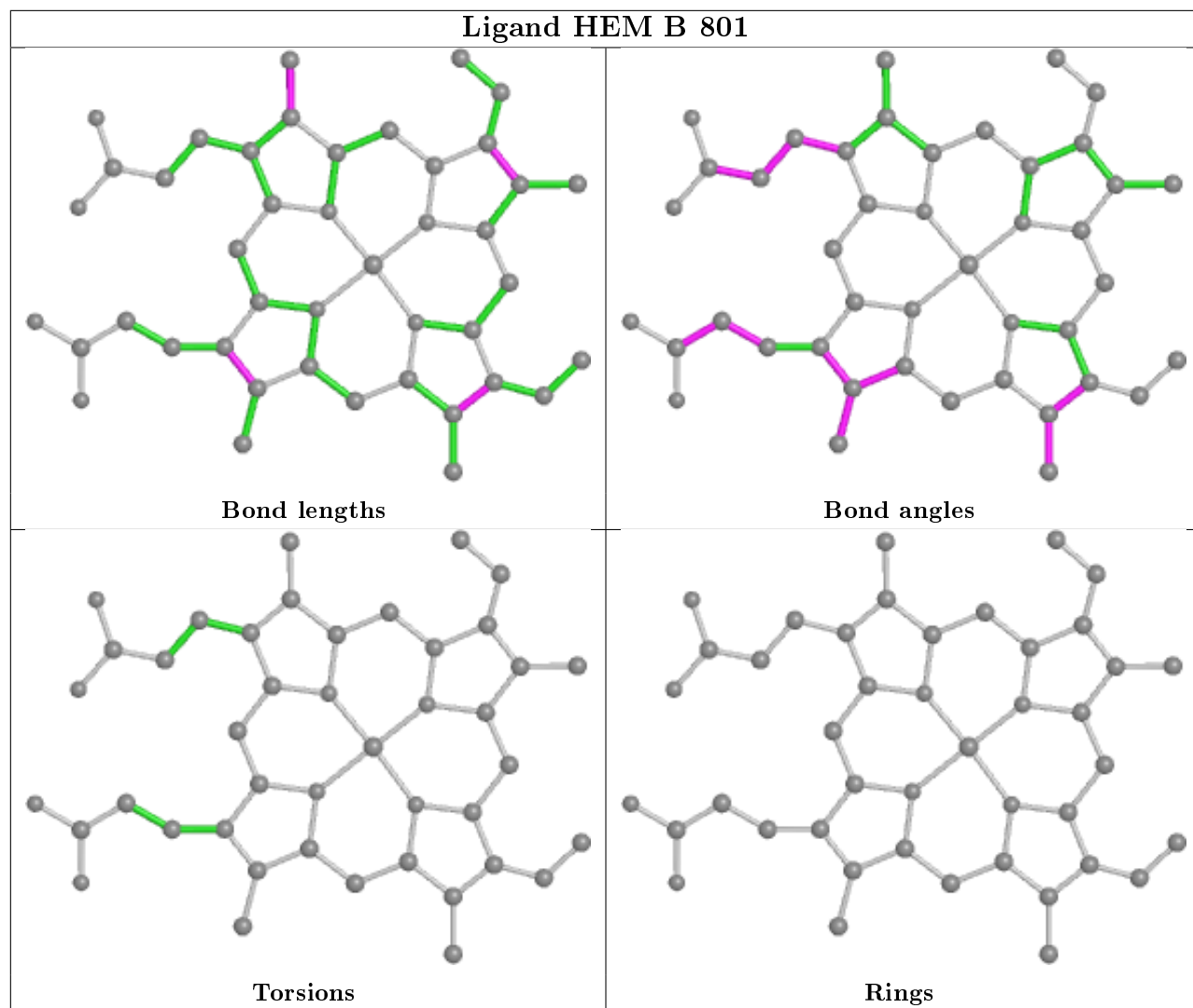
Mol	Chain	Res	Type	Atoms
7	B	807	MPD	C1-C2-C3-C4
7	B	807	MPD	O2-C2-C3-C4
7	B	808	MPD	O2-C2-C3-C4
7	B	808	MPD	CM-C2-C3-C4
7	B	807	MPD	CM-C2-C3-C4

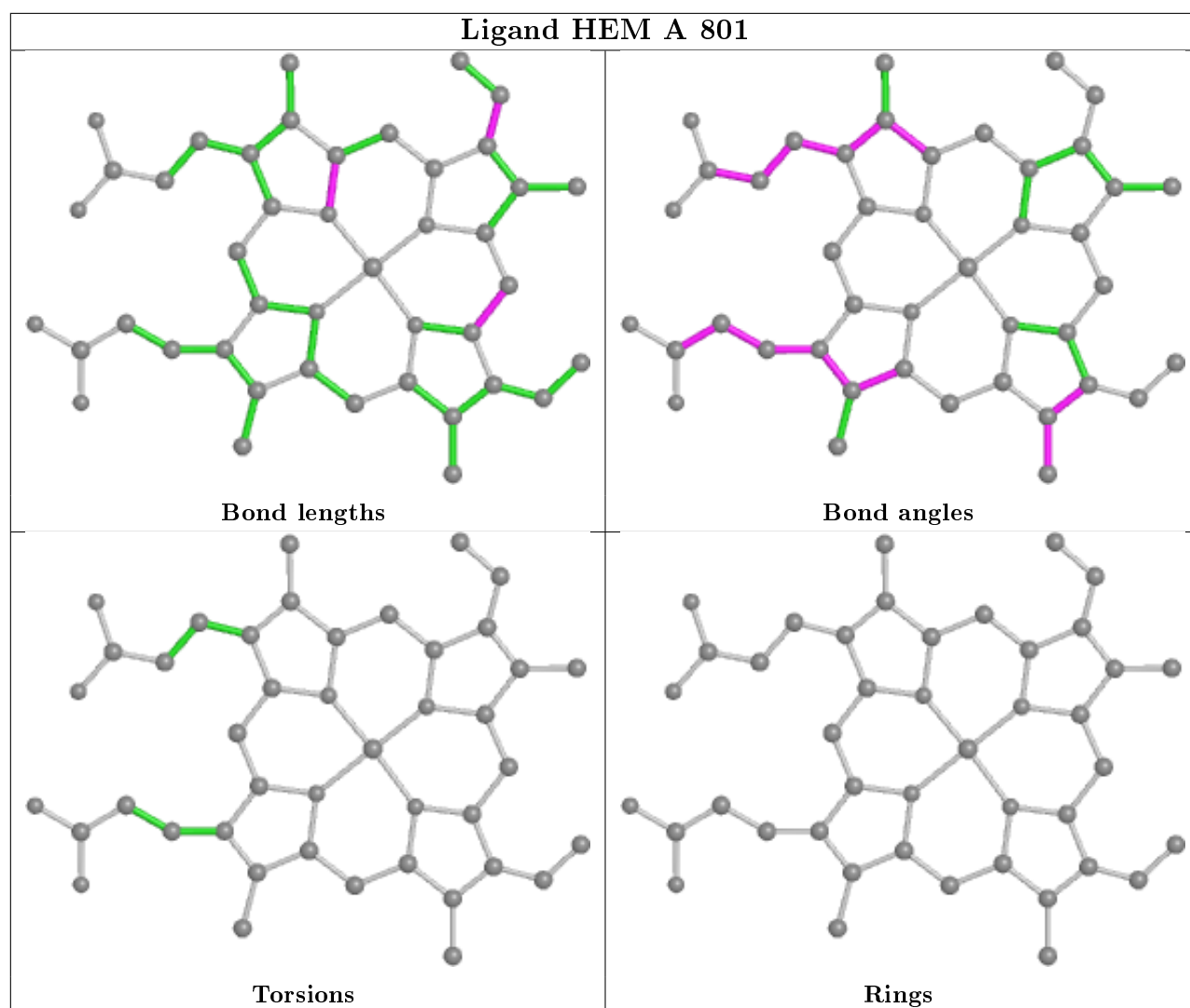
There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	807	MPD	1	0
8	A	809	NIZ	2	0
5	B	805	OXY	1	0
7	A	808	MPD	1	0
7	A	807	MPD	2	0
8	B	809	NIZ	1	0
2	A	801	HEM	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	713/728 (97%)	-0.51	7 (0%) 82 83	12, 18, 35, 74	0
1	B	713/728 (97%)	-0.53	6 (0%) 86 87	12, 17, 34, 67	0
All	All	1426/1456 (97%)	-0.52	13 (0%) 84 85	12, 18, 34, 74	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748	ALA	4.2
1	A	541	GLY	4.0
1	A	540	ARG	3.5
1	B	748	ALA	3.4
1	A	679	ALA	3.3

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 carbohydrates in this entry.

6.4 Ligands [i](#)

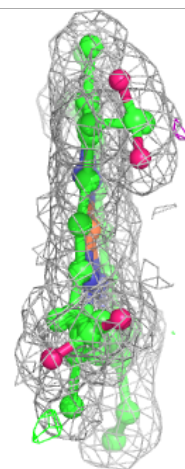
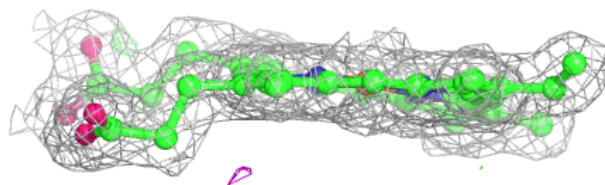
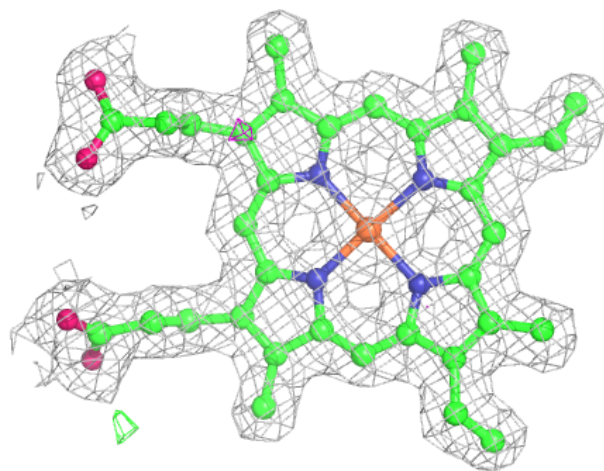
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

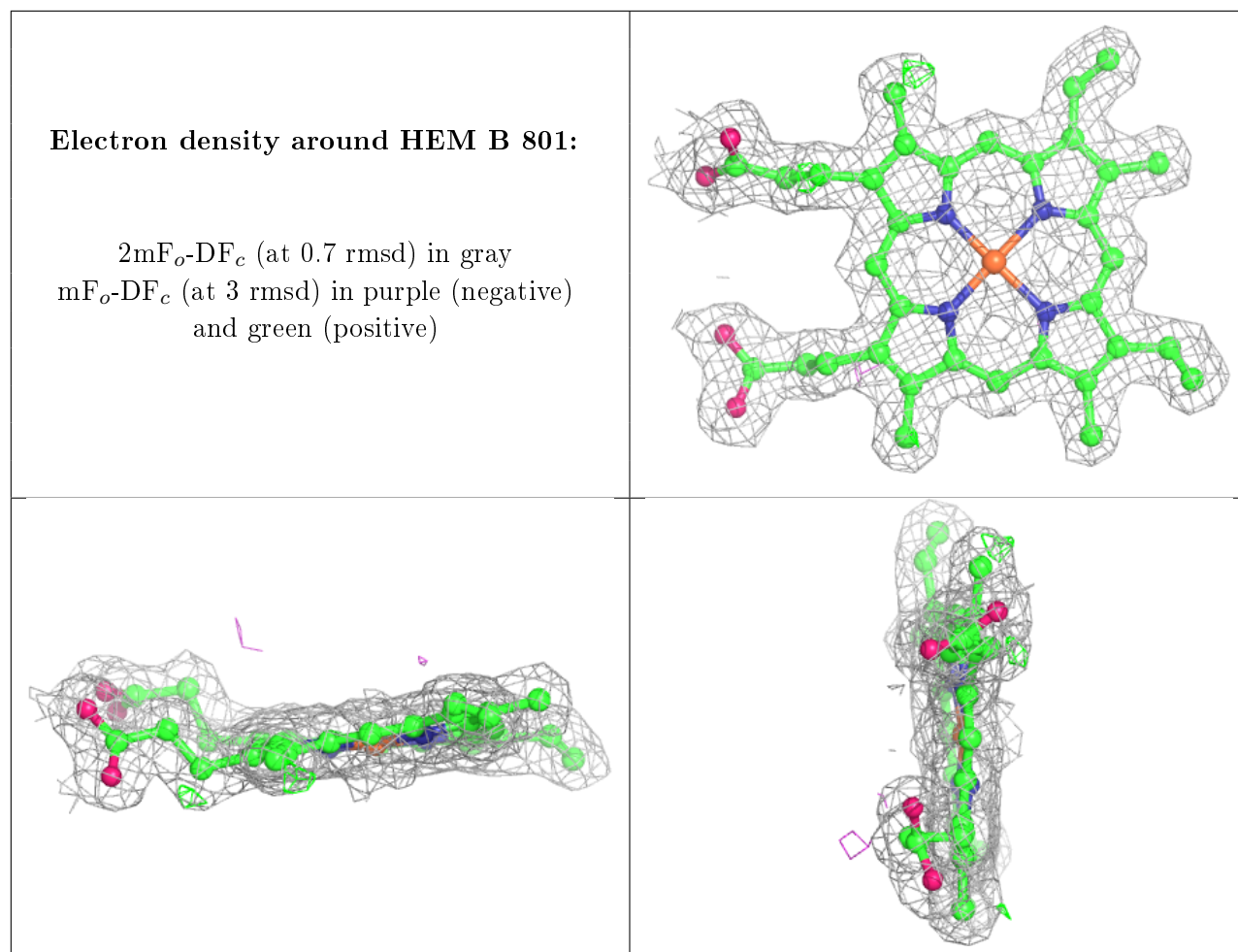
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	NIZ	A	809	10/10	0.81	0.45	17,20,22,24	10
8	NIZ	B	809	10/10	0.91	0.13	21,24,29,29	10
7	MPD	A	808	8/8	0.93	0.14	35,40,54,56	0
7	MPD	B	807	8/8	0.93	0.14	39,42,47,48	0
7	MPD	B	808	8/8	0.93	0.12	40,43,45,47	0
6	PO4	A	806	5/5	0.94	0.14	40,50,59,59	0
7	MPD	A	807	8/8	0.95	0.14	50,58,59,64	0
6	PO4	B	806	5/5	0.95	0.21	39,50,56,61	0
5	OXY	B	805	2/2	0.95	0.10	31,31,31,39	0
5	OXY	A	805	2/2	0.97	0.10	32,32,32,38	0
5	OXY	B	804	2/2	0.99	0.10	24,24,24,27	0
4	CL	B	803	1/1	0.99	0.07	23,23,23,23	0
3	NA	A	802	1/1	0.99	0.06	15,15,15,15	0
4	CL	A	803	1/1	0.99	0.07	25,25,25,25	0
5	OXY	A	804	2/2	0.99	0.16	25,25,25,33	0
2	HEM	A	801	43/43	0.99	0.07	12,14,17,18	0
2	HEM	B	801	43/43	0.99	0.09	12,13,14,15	0
3	NA	B	802	1/1	1.00	0.04	14,14,14,14	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 A 801:

$2mF_o-DF_c$ (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.