



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:19 PM UTC

PDB ID : 5KT9 / pdb_00005kt9
Title : Crystal structure of the catalase-peroxidase from *B. pseudomallei* treated with hydrogen peroxide and carbon monoxide
Authors : Loewen, P.C.
Deposited on : 2016-07-11
Resolution : 1.88 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

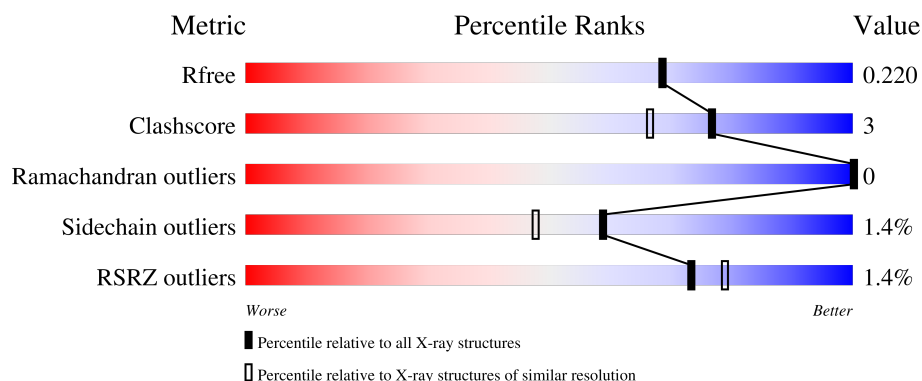
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	728	0% 84% 13% ..
1	B	728	2% 83% 15% ..

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
6	MPD	B	802	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12633 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 Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total	C	N	O	S	0	5	0
			5532	3493	985	1040	14			
1	B	713	Total	C	N	O	S	0	9	0
			5552	3508	990	1040	14			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: 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		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

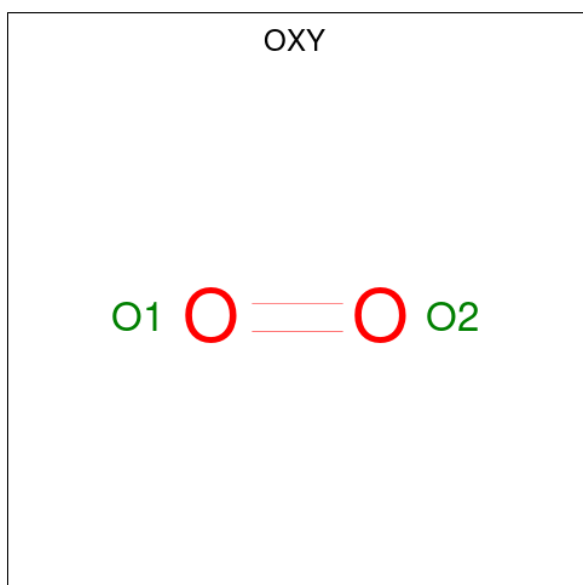
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 5 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



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

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	726	Total	O	0	0
			726	726		
7	B	689	Total	O	0	0
			689	689		

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.

Chain A:

Residue	Percentage	Color
MET	84%	Green
SER	84%	Green
ASN	84%	Green
GLU	84%	Green
ALA	84%	Green
LYS	84%	Green
CYS	84%	Green
PRO	84%	Green
PHE	84%	Green
HIS	84%	Green
GLN	84%	Green
ALA	84%	Green
ALA	84%	Green
GLY	84%	Green
ASN	84%	Green
G36	84%	Green
R40	84%	Yellow
Q46	84%	Yellow
L47	84%	Yellow
D48	84%	Yellow
L49	84%	Yellow
S50	84%	Yellow
I51	84%	Yellow
L52	84%	Yellow
H53	84%	Yellow
R54	84%	Yellow
H55	84%	Yellow
K64	84%	Orange
Y68	84%	Yellow
A69	84%	Yellow
Q70	84%	Yellow
E73	84%	Yellow
L87	84%	Yellow
M88	84%	Yellow
S91	84%	Yellow
Q92	84%	Yellow
D93	84%	Yellow
W94	84%	Yellow
W95	84%	Yellow
Y102	84%	Yellow
I107	84%	Yellow
TOX111	84%	Yellow
G115	84%	Yellow
T119	84%	Yellow
A126	84%	Yellow
T141	84%	Yellow
R150	84%	Yellow
D127	84%	Yellow
P154	84%	Yellow
A166	84%	Yellow
V175	84%	Yellow
G186	84%	Yellow
P197	84%	Yellow
G203	84%	Yellow
V232	84%	Yellow
G243	84%	Yellow
N247	84%	Yellow
R255	84%	Yellow
M264	84%	Yellow
A265	84%	Yellow
M266	84%	Yellow
E269	84%	Yellow
E270	84%	Yellow
T271	84%	Yellow
N292	84%	Yellow
A295	84%	Yellow
K310	84%	Yellow
W330	84%	Yellow
T333	84%	Yellow
E343	84%	Orange
A364	84%	Yellow
K365	84%	Yellow
A374	84%	Yellow
S402	84%	Yellow
R403	84%	Yellow
R404	84%	Yellow
F412	84%	Yellow
A413	84%	Yellow
D414	84%	Yellow
A415	84%	Yellow
F416	84%	Green
A417	84%	Yellow
R418	84%	Yellow
R426	84%	Yellow
M428	84%	Orange
R431	84%	Yellow
A432	84%	Green
R433	84%	Yellow
E438	84%	Yellow
Q447	84%	Yellow
P451	84%	Yellow
H455	84%	Yellow
L466	84%	Orange
V470	84%	Yellow
V477	84%	Yellow
L480	84%	Yellow
V481	84%	Yellow
W485	84%	Yellow
G499	84%	Yellow
E529	84%	Yellow
R532	84%	Yellow
R540	84%	Yellow
C556	84%	Yellow
V559	84%	Yellow
E560	84%	Yellow
H568	84%	Yellow
V572	84%	Yellow
T586	84%	Yellow
V593	84%	Yellow
L605	84%	Yellow
K608	84%	Orange
Y609	84%	Yellow
R610	84%	Yellow
V611	84%	Green
P612	84%	Yellow
A613	84%	Yellow
L616	84%	Yellow
L617	84%	Yellow
V618	84%	Yellow

Chain B:

83% 15% 2%

MET SER ASN GLU ALA LYS CYS PRO PHE HIS GLN ALA ALA GLY ASN G36 R40 Q46 L47 D48 I51 L52 H53 R54 H55 L58 P61 M62 G63 K64 D65 K74 S91 Q92 D93 Y94 H101 I107 T107 T116 Y117 R118 T119 L136 R137 S138 D141 M142 D146 R149 W153 F154 I155 K156 Q157 L168 V175 E178 F182 K183 A192 E198 D199 N240 N264 A265 T271 L274 G278 H285 G288 A296 E298 K310 I322 N340 F342 K365 K380 H381 R382 E399 H406 F412 A413 D414 A415 F416 A417 R418 A419 M428 R431 A432 R433 V439 Q447 D448 P449 I450 L475 Q479 L480 W485 R504 F505 R506 D512 Q520 E526 T527 R540 C556 A575 T586 M591 A592 V593 L594 L605 R610 V618 D619 K620 L626 P629 V633 V645 G646 Q647 E657 N662 D663 F664 A679 A680 R688 E694 S708 R713 E717 V718 Y719 D723 A724 Q725 E726 R730 D746 L747 A748

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.85Å 113.79Å 174.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.88 50.00 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-1.88) 99.2 (50.00-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.177 , 0.213 0.187 , 0.220	Depositor DCC
R_{free} test set	8088 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.920	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12633	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: HEM, NA, TOX, CL, MPD, OXY

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	1.78	66/5666 (1.2%)	1.30	13/7700 (0.2%)
1	B	1.75	66/5700 (1.2%)	1.31	18/7745 (0.2%)
All	All	1.77	132/11366 (1.2%)	1.30	31/15445 (0.2%)

All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	117	TYR	C-O	-8.44	1.13	1.23
1	B	94	TRP	C-O	-8.12	1.13	1.24
1	B	475	LEU	C-O	-8.09	1.14	1.23
1	B	708	SER	CA-C	-8.04	1.45	1.52
1	A	413	ALA	N-CA	7.92	1.55	1.46
1	A	499	GLY	C-O	7.81	1.32	1.24
1	A	186	GLY	N-CA	7.79	1.53	1.45
1	B	527	THR	N-CA	-7.54	1.37	1.46
1	A	271	THR	N-CA	7.45	1.55	1.46
1	B	91	SER	C-O	-7.35	1.15	1.23
1	A	403	ARG	CD-NE	7.33	1.56	1.46
1	B	645	VAL	N-CA	7.20	1.55	1.46
1	B	271	THR	N-CA	7.09	1.54	1.46
1	B	107	ILE	N-CA	7.07	1.54	1.46
1	B	182	PHE	C-O	-6.98	1.15	1.24
1	A	197	PRO	CA-C	-6.93	1.43	1.52
1	B	149	ARG	N-CA	-6.90	1.38	1.46
1	A	605	LEU	C-O	-6.86	1.15	1.24
1	B	310	LYS	C-O	-6.82	1.15	1.23
1	A	87	LEU	N-CA	-6.81	1.38	1.46
1	A	612	PRO	CA-C	6.81	1.60	1.52
1	B	439	VAL	C-O	-6.79	1.15	1.24
1	B	156	LYS	CA-CB	-6.79	1.42	1.53
1	B	726	GLU	CD-OE1	6.79	1.38	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	725	GLN	CG-CD	6.74	1.69	1.52
1	A	556	CYS	N-CA	6.73	1.54	1.46
1	A	732	PHE	N-CA	6.72	1.54	1.46
1	A	618	VAL	CA-CB	6.69	1.63	1.54
1	A	532	ARG	NE-CZ	-6.62	1.25	1.33
1	A	88	MET	C-O	-6.58	1.16	1.24
1	A	175	VAL	N-CA	-6.53	1.37	1.46
1	A	92	GLN	CA-C	6.52	1.60	1.52
1	A	634	LEU	N-CA	-6.48	1.38	1.46
1	B	142	ASN	N-CA	6.48	1.54	1.46
1	A	623	LEU	N-CA	-6.45	1.38	1.46
1	B	298	GLU	C-O	-6.43	1.15	1.24
1	A	417	ALA	N-CA	6.42	1.54	1.46
1	A	616	LEU	N-CA	-6.40	1.38	1.46
1	B	342	PHE	C-O	6.38	1.32	1.24
1	B	620	LYS	CA-C	6.33	1.60	1.52
1	A	232	VAL	N-CA	6.31	1.54	1.46
1	B	155	ILE	C-O	6.25	1.31	1.24
1	B	240	ASN	C-O	6.18	1.32	1.24
1	A	620	LYS	C-O	-6.17	1.17	1.24
1	A	485	TRP	N-CA	6.17	1.53	1.46
1	B	485	TRP	N-CA	6.16	1.53	1.46
1	A	418	ARG	CA-C	-6.12	1.45	1.52
1	A	87	LEU	C-O	6.11	1.31	1.24
1	A	365	LYS	N-CA	6.09	1.53	1.46
1	B	340	ASN	N-CA	-6.07	1.38	1.46
1	B	417	ALA	N-CA	6.04	1.53	1.46
1	B	36	GLY	N-CA	5.99	1.55	1.45
1	B	285	HIS	N-CA	5.99	1.53	1.46
1	A	415	ALA	C-N	-5.98	1.25	1.33
1	B	199	ASP	CA-C	-5.93	1.45	1.52
1	B	620	LYS	CA-CB	-5.93	1.44	1.53
1	A	68	TYR	CA-CB	5.92	1.62	1.53
1	B	415	ALA	CA-CB	5.92	1.62	1.53
1	A	737	ASN	N-CA	-5.91	1.39	1.46
1	A	455	HIS	C-O	-5.91	1.18	1.24
1	A	330	TRP	N-CA	5.88	1.53	1.46
1	B	717	GLU	N-CA	-5.88	1.38	1.46
1	B	168	LEU	CA-C	5.84	1.60	1.52
1	B	512	ASP	CG-OD2	5.84	1.36	1.25
1	A	559	VAL	CA-C	5.84	1.60	1.52
1	B	413	ALA	N-CA	5.84	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	166	ALA	N-CA	5.83	1.53	1.46
1	B	723	ASP	C-O	-5.76	1.16	1.24
1	A	477	VAL	CA-C	5.75	1.60	1.52
1	A	710	SER	C-O	5.71	1.31	1.24
1	B	657	GLU	CA-C	5.70	1.59	1.52
1	B	92	GLN	CA-C	5.69	1.60	1.52
1	B	586	THR	C-O	5.69	1.30	1.23
1	A	650	HIS	CA-CB	-5.69	1.45	1.53
1	A	731	ASP	N-CA	-5.68	1.39	1.46
1	A	572	VAL	C-O	-5.65	1.16	1.24
1	B	746	ASP	C-O	-5.63	1.16	1.24
1	B	399	GLU	CA-CB	5.62	1.62	1.53
1	A	480	LEU	N-CA	-5.60	1.39	1.46
1	B	556	CYS	N-CA	5.58	1.53	1.46
1	B	365	LYS	N-CA	5.56	1.52	1.46
1	A	613	ALA	C-O	-5.53	1.17	1.24
1	B	626	LEU	C-O	5.53	1.30	1.23
1	A	560	GLU	N-CA	5.53	1.53	1.46
1	A	540	ARG	C-O	5.50	1.30	1.23
1	A	95	TRP	N-CA	5.50	1.52	1.46
1	B	295	ALA	C-O	-5.50	1.17	1.23
1	A	107	ILE	N-CA	5.49	1.52	1.46
1	B	449	PRO	N-CA	-5.49	1.40	1.47
1	A	154	PRO	C-O	-5.44	1.17	1.24
1	A	102	TYR	CA-CB	-5.42	1.44	1.53
1	A	333	THR	N-CA	5.41	1.52	1.46
1	B	157	GLN	N-CA	-5.40	1.39	1.46
1	B	274	LEU	CA-C	-5.40	1.45	1.52
1	B	419	ALA	N-CA	-5.40	1.39	1.46
1	A	266	MET	CA-CB	-5.39	1.45	1.53
1	B	575	ALA	N-CA	5.39	1.53	1.46
1	A	733	VAL	CA-CB	5.37	1.61	1.54
1	B	101	HIS	N-CA	5.32	1.52	1.46
1	A	415	ALA	CA-C	5.30	1.59	1.52
1	A	150	ARG	C-O	5.30	1.30	1.24
1	B	153	TRP	CA-CB	5.29	1.61	1.53
1	A	374	ALA	C-O	5.26	1.30	1.24
1	B	480	LEU	N-CA	-5.25	1.40	1.46
1	A	292	ASN	CA-C	5.25	1.59	1.52
1	B	138	SER	CA-C	-5.24	1.46	1.52
1	A	203	GLY	C-O	5.24	1.28	1.23
1	B	175	VAL	N-CA	-5.23	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	ALA	CA-C	-5.23	1.45	1.52
1	A	438	GLU	CA-C	-5.22	1.46	1.52
1	B	198	GLU	CD-OE2	5.21	1.35	1.25
1	B	341	PHE	CA-C	5.21	1.59	1.52
1	B	526	GLU	N-CA	5.20	1.52	1.46
1	A	706	PHE	CA-CB	5.20	1.62	1.53
1	A	402	SER	CA-CB	5.17	1.61	1.53
1	A	295	ALA	CA-C	5.16	1.59	1.52
1	B	101	HIS	CA-C	5.14	1.58	1.52
1	B	322	ILE	N-CA	-5.14	1.39	1.46
1	A	414	ASP	N-CA	-5.13	1.40	1.46
1	B	688	ARG	CA-C	-5.13	1.46	1.52
1	A	586	THR	C-O	5.13	1.29	1.24
1	A	310	LYS	C-O	-5.10	1.17	1.23
1	A	91	SER	N-CA	5.09	1.52	1.46
1	B	664	PHE	N-CA	-5.07	1.40	1.46
1	A	481	VAL	N-CA	5.05	1.52	1.46
1	B	605	LEU	C-O	-5.04	1.18	1.24
1	B	480	LEU	C-N	-5.03	1.27	1.33
1	B	146	ASP	C-O	5.01	1.29	1.24
1	B	192	ALA	N-CA	5.01	1.52	1.46
1	B	61	PRO	C-O	-5.01	1.18	1.24
1	A	451	PRO	C-O	5.00	1.29	1.23
1	B	619	ASP	C-O	-5.00	1.18	1.24

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	62	MET	CA-C-N	-8.23	111.47	120.44
1	B	62	MET	C-N-CA	-8.23	111.47	120.44
1	B	479	GLN	N-CA-C	7.82	120.50	111.11
1	B	428	MET	CA-CB-CG	-6.91	100.29	114.10
1	B	450	ILE	N-CA-CB	-6.50	104.65	111.61
1	A	412	PHE	N-CA-C	-6.46	104.16	111.14
1	A	93	ASP	N-CA-C	6.38	119.05	111.71
1	B	55	HIS	CB-CA-C	6.28	120.17	111.63
1	A	48	ASP	N-CA-C	6.22	119.00	107.99
1	A	343	GLU	CB-CG-CD	6.08	122.94	112.60
1	B	713	ARG	NE-CZ-NH1	6.00	127.50	121.50
1	A	46	GLN	CB-CG-CD	5.95	122.72	112.60
1	B	412	PHE	N-CA-C	-5.80	104.86	111.07
1	A	270	GLU	N-CA-C	-5.78	104.95	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	428	MET	CA-CB-CG	-5.72	102.65	114.10
1	A	364	ALA	CA-C-O	-5.70	115.20	121.58
1	B	58	LEU	N-CA-C	5.49	116.95	111.07
1	B	48	ASP	N-CA-C	5.43	117.60	107.99
1	B	708	SER	N-CA-C	5.39	119.35	112.12
1	B	620	LYS	N-CA-C	-5.36	105.35	111.14
1	A	529	GLU	CB-CG-CD	5.33	121.67	112.60
1	A	343	GLU	CA-CB-CG	5.32	124.74	114.10
1	B	288	GLY	CA-C-N	5.32	125.33	119.90
1	B	288	GLY	C-N-CA	5.32	125.33	119.90
1	B	450	ILE	CB-CA-C	-5.26	104.74	110.37
1	A	365	LYS	N-CA-C	5.17	116.91	111.28
1	A	64	LYS	CB-CG-CD	5.15	123.15	111.30
1	A	466	LEU	N-CA-C	5.15	116.89	111.28
1	B	278	GLY	N-CA-C	5.12	118.84	112.64
1	B	428	MET	N-CA-C	5.09	119.20	112.89
1	B	136	LEU	CA-C-O	5.01	125.74	119.97

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	5532	0	5345	22	0
1	B	5552	0	5384	31	0
2	A	43	0	30	0	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	2	0	0	0	0
5	B	2	0	0	0	0
6	A	16	0	28	3	0
6	B	24	0	42	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	726	0	0	7	0
7	B	689	0	0	10	0
All	All	12633	0	10859	63	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 3.

All (63) 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:B:53:HIS:NE2	7:B:902:HOH:O	2.09	0.85
1:A:119[B]:THR:HG21	7:A:1195:HOH:O	1.78	0.84
1:B:506:ARG:HE	6:B:802:MPD:H12	1.43	0.83
1:A:54:ARG:O	7:A:901:HOH:O	2.01	0.79
1:B:119[B]:THR:HG22	1:B:593:VAL:HG21	1.65	0.77
1:B:55:HIS:HD2	7:B:1228:HOH:O	1.67	0.76
6:B:802:MPD:H51	7:B:1227:HOH:O	1.86	0.75
1:B:119[B]:THR:HG23	7:B:1054:HOH:O	1.88	0.74
6:A:806:MPD:O4	6:A:806:MPD:O2	2.07	0.69
6:B:802:MPD:H13	7:B:1491:HOH:O	1.93	0.67
1:B:540:ARG:HA	1:B:540:ARG:NH1	2.13	0.64
1:B:629:PRO:O	1:B:633[A]:VAL:HG23	1.98	0.63
1:B:540:ARG:HA	1:B:540:ARG:CZ	2.28	0.63
1:A:70[A]:GLN:NE2	7:A:905:HOH:O	2.29	0.59
6:B:807:MPD:O4	6:B:807:MPD:C1	2.50	0.59
1:B:662:ASN:H	1:B:725:GLN:HE22	1.52	0.57
1:B:730[A]:ARG:HD2	7:B:1413:HOH:O	2.05	0.56
1:A:269:GLU:OE1	1:A:404:ARG:NH2	2.29	0.56
1:A:119[B]:THR:HG23	1:A:593:VAL:HG11	1.87	0.55
1:B:506:ARG:HE	6:B:802:MPD:C1	2.17	0.55
1:A:568:HIS:CD2	1:A:725:GLN:OE1	2.60	0.55
6:B:806:MPD:O4	6:B:806:MPD:HM2	2.05	0.55
1:A:269:GLU:HG2	7:A:1467:HOH:O	2.08	0.53
1:A:343:GLU:HG3	7:A:1471:HOH:O	2.09	0.53
1:A:50:SER:HA	1:A:53:HIS:CE1	2.44	0.52
6:B:802:MPD:C1	6:B:802:MPD:H52	2.40	0.52
1:B:428:MET:O	1:B:433:ARG:HD3	2.10	0.50
1:A:426:ARG:HG3	1:A:426:ARG:O	2.10	0.50
1:B:382:ARG:HD2	7:B:920:HOH:O	2.10	0.50
1:A:428:MET:O	1:A:433:ARG:HD3	2.12	0.49
1:B:591:MET:SD	1:B:594:LEU:HD12	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ILE:HD11	1:A:618:VAL:HG12	1.94	0.49
1:B:633[A]:VAL:HG22	1:B:719:TYR:CZ	2.48	0.48
6:A:805:MPD:H11	6:A:805:MPD:C5	2.43	0.48
1:B:629:PRO:O	1:B:633[B]:VAL:HG12	2.14	0.47
1:B:51:ILE:HD11	1:B:618:VAL:HG12	1.96	0.47
1:A:255[A]:ARG:HG2	7:A:908:HOH:O	2.14	0.47
1:A:47:LEU:O	7:A:902:HOH:O	2.21	0.46
1:B:633[A]:VAL:HG22	1:B:719:TYR:CE2	2.51	0.46
1:B:178:GLU:OE1	7:B:903:HOH:O	2.21	0.45
1:A:115:GLY:O	1:A:264:MET:HE1	2.17	0.45
1:B:520[B]:GLN:OE1	1:B:647:GLN:NE2	2.49	0.45
6:A:805:MPD:H11	6:A:805:MPD:H53	1.98	0.45
1:A:466:LEU:O	1:A:470:VAL:HG23	2.17	0.44
1:B:406:HIS:HE1	7:B:1457:HOH:O	1.99	0.44
1:A:431:ARG:HD2	1:A:447:GLN:OE1	2.18	0.44
6:B:802:MPD:H12	6:B:802:MPD:H52	1.99	0.44
1:B:264:MET:O	1:B:265:ALA:HB3	2.18	0.44
1:B:115:GLY:O	1:B:264:MET:SD	2.77	0.43
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	3.02	0.43
1:A:264:MET:O	1:A:265:ALA:HB3	2.18	0.43
1:B:183:LYS:HD2	7:B:1014:HOH:O	2.19	0.43
6:B:806:MPD:O4	6:B:806:MPD:CM	2.66	0.43
1:B:115:GLY:O	1:B:264:MET:HE1	2.18	0.42
1:B:504:ARG:HD3	1:B:591:MET:HE3	2.01	0.42
1:B:51:ILE:HD13	1:B:51:ILE:HG21	1.89	0.42
1:A:115:GLY:O	1:A:264:MET:SD	2.78	0.41
1:B:431:ARG:HD2	1:B:447:GLN:OE1	2.20	0.41
1:A:243:GLY:HA3	1:A:247:ASN:O	2.21	0.41
1:B:119[B]:THR:HG22	1:B:593:VAL:HG11	2.03	0.41
1:A:706:PHE:O	1:A:713:ARG:HA	2.20	0.40
1:A:119[B]:THR:CG2	1:A:593:VAL:HG11	2.51	0.40
1:B:74:LYS:HA	1:B:74:LYS:HE2	2.04	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	A	714/728 (98%)	703 (98%)	11 (2%)	0	100	100
1	B	718/728 (99%)	708 (99%)	10 (1%)	0	100	100
All	All	1432/1456 (98%)	1411 (98%)	21 (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	A	553/560 (99%)	548 (99%)	5 (1%)	70	63
1	B	557/560 (100%)	546 (98%)	11 (2%)	48	33
All	All	1110/1120 (99%)	1094 (99%)	16 (1%)	59	48

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	64	LYS
1	A	73	GLU
1	A	141	ASP
1	A	610	ARG
1	B	40	ARG
1	B	46	GLN
1	B	64	LYS
1	B	74	LYS
1	B	141	ASP
1	B	380	LYS
1	B	540	ARG
1	B	610	ARG
1	B	633[A]	VAL

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Mol	Chain	Res	Type
1	B	633[B]	VAL
1	B	694	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	53	HIS
1	A	539	GLN
1	A	544	GLN
1	A	568	HIS
1	A	647	GLN
1	B	53	HIS
1	B	55	HIS
1	B	224	GLN
1	B	647	GLN
1	B	650	HIS
1	B	725	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
1	TOX	A	111[A]	2	14,17,18	2.81	6 (42%)	12,23,25	2.62	6 (50%)
1	TOX	B	111[B]	-	14,17,18	2.06	4 (28%)	12,23,25	2.62	7 (58%)
1	TOX	B	111[A]	-	14,17,18	2.06	4 (28%)	12,23,25	2.62	7 (58%)
1	TOX	A	111[B]	-	14,17,18	2.81	6 (42%)	12,23,25	2.62	6 (50%)

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
1	TOX	A	111[A]	2	-	2/5/8/10	0/2/2/2
1	TOX	B	111[B]	-	-	2/5/8/10	0/2/2/2
1	TOX	B	111[A]	-	-	2/5/8/10	0/2/2/2
1	TOX	A	111[B]	-	-	2/5/8/10	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111[A]	TOX	CD2-CE2	6.17	1.49	1.41
1	A	111[B]	TOX	CD2-CE2	6.17	1.49	1.41
1	B	111[A]	TOX	O-C	5.26	1.40	1.20
1	B	111[B]	TOX	O-C	5.26	1.40	1.20
1	A	111[A]	TOX	O-C	4.71	1.37	1.20
1	A	111[B]	TOX	O-C	4.71	1.37	1.20
1	A	111[A]	TOX	CE2-NE1	-4.36	1.32	1.39
1	A	111[B]	TOX	CE2-NE1	-4.36	1.32	1.39
1	A	111[A]	TOX	CE3-CD2	-3.03	1.35	1.39
1	A	111[B]	TOX	CE3-CD2	-3.03	1.35	1.39
1	A	111[A]	TOX	CH2-CZ3	2.91	1.44	1.38
1	A	111[B]	TOX	CH2-CZ3	2.91	1.44	1.38
1	B	111[A]	TOX	CD2-CE2	2.63	1.44	1.41
1	B	111[B]	TOX	CD2-CE2	2.63	1.44	1.41
1	A	111[A]	TOX	CD1-CG	2.50	1.41	1.36
1	A	111[B]	TOX	CD1-CG	2.50	1.41	1.36
1	B	111[A]	TOX	CH2-CZ3	2.38	1.43	1.38
1	B	111[B]	TOX	CH2-CZ3	2.38	1.43	1.38
1	B	111[A]	TOX	CZ2-CE2	-2.32	1.36	1.39
1	B	111[B]	TOX	CZ2-CE2	-2.32	1.36	1.39

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111[A]	TOX	CZ2-CE2-CD2	-5.22	116.12	121.95
1	A	111[B]	TOX	CZ2-CE2-CD2	-5.22	116.12	121.95
1	B	111[A]	TOX	CZ2-CE2-NE1	4.81	137.04	129.37
1	B	111[B]	TOX	CZ2-CE2-NE1	4.81	137.04	129.37
1	B	111[A]	TOX	CZ3-CH2-CZ2	-4.65	114.50	120.24
1	B	111[B]	TOX	CZ3-CH2-CZ2	-4.65	114.50	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111[A]	TOX	CE3-CD2-CE2	4.10	123.97	119.24
1	A	111[B]	TOX	CE3-CD2-CE2	4.10	123.97	119.24
1	A	111[A]	TOX	CZ2-CE2-NE1	3.62	135.14	129.37
1	A	111[B]	TOX	CZ2-CE2-NE1	3.62	135.14	129.37
1	B	111[A]	TOX	CB-CG-CD1	-3.07	122.41	126.67
1	B	111[B]	TOX	CB-CG-CD1	-3.07	122.41	126.67
1	A	111[A]	TOX	CD2-CG-CD1	-2.96	103.66	106.34
1	A	111[B]	TOX	CD2-CG-CD1	-2.96	103.66	106.34
1	B	111[A]	TOX	CH2-CZ2-CE2	2.95	124.23	118.28
1	B	111[B]	TOX	CH2-CZ2-CE2	2.95	124.23	118.28
1	B	111[A]	TOX	CH2-CZ3-CE3	2.62	123.48	120.24
1	B	111[B]	TOX	CH2-CZ3-CE3	2.62	123.48	120.24
1	B	111[A]	TOX	CZ2-CE2-CD2	-2.40	119.28	121.95
1	B	111[B]	TOX	CZ2-CE2-CD2	-2.40	119.28	121.95
1	A	111[A]	TOX	CE3-CD2-CG	-2.20	130.57	133.85
1	A	111[B]	TOX	CE3-CD2-CG	-2.20	130.57	133.85
1	A	111[A]	TOX	CE2-CD2-CG	-2.17	105.40	107.39
1	A	111[B]	TOX	CE2-CD2-CG	-2.17	105.40	107.39
1	B	111[A]	TOX	CB-CG-CD2	2.12	130.76	126.70
1	B	111[B]	TOX	CB-CG-CD2	2.12	130.76	126.70

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	111[A]	TOX	N-CA-CB-CG
1	A	111[A]	TOX	C-CA-CB-CG
1	A	111[B]	TOX	N-CA-CB-CG
1	A	111[B]	TOX	C-CA-CB-CG
1	B	111[A]	TOX	N-CA-CB-CG
1	B	111[A]	TOX	C-CA-CB-CG
1	B	111[B]	TOX	N-CA-CB-CG
1	B	111[B]	TOX	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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
6	MPD	B	807	-	7,7,7	0.75	0	9,10,10	1.04	0
6	MPD	B	802	-	7,7,7	0.97	0	9,10,10	1.56	2 (22%)
6	MPD	B	806	-	7,7,7	0.77	0	9,10,10	0.80	0
6	MPD	A	806	-	7,7,7	1.02	1 (14%)	9,10,10	2.57	6 (66%)
2	HEM	A	801	1	50,50,50	2.04	14 (28%)	67,82,82	1.96	24 (35%)
5	OXY	B	805	-	1,1,1	0.31	0	-	-	-
5	OXY	A	804	-	1,1,1	0.11	0	-	-	-
6	MPD	A	805	-	7,7,7	0.55	0	9,10,10	1.56	3 (33%)
2	HEM	B	801	1	50,50,50	1.78	16 (32%)	67,82,82	1.73	17 (25%)

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
6	MPD	B	807	-	-	4/5/5/5	-
6	MPD	B	802	-	-	2/5/5/5	-
6	MPD	B	806	-	-	4/5/5/5	-
6	MPD	A	806	-	-	1/5/5/5	-
2	HEM	A	801	1	-	2/14/54/54	-
6	MPD	A	805	-	-	3/5/5/5	-
2	HEM	B	801	1	-	2/14/54/54	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	FE-NB	6.05	2.13	1.94
2	A	801	HEM	C4D-ND	-4.46	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	FE-NB	4.29	2.08	1.94
2	B	801	HEM	C4A-NA	-4.07	1.32	1.39
2	A	801	HEM	C4B-NB	-4.04	1.30	1.38
2	A	801	HEM	FE-NC	3.77	2.07	1.95
2	A	801	HEM	FE-NA	3.71	2.07	1.95
2	A	801	HEM	C1B-NB	-3.70	1.33	1.40
2	A	801	HEM	O1D-CGD	3.62	1.33	1.22
2	B	801	HEM	C1B-NB	-3.58	1.34	1.40
2	B	801	HEM	C1C-NC	-3.55	1.32	1.39
2	B	801	HEM	FE-NA	3.33	2.06	1.95
2	A	801	HEM	CHA-C4D	-3.19	1.32	1.38
2	B	801	HEM	C3C-C2C	2.90	1.43	1.37
2	A	801	HEM	C1D-ND	-2.86	1.33	1.38
2	B	801	HEM	CMC-C2C	2.79	1.56	1.50
2	B	801	HEM	CHA-C4D	-2.52	1.33	1.38
2	A	801	HEM	C3C-C2C	2.41	1.42	1.37
2	B	801	HEM	C4C-NC	2.40	1.44	1.39
2	B	801	HEM	C1D-C2D	-2.24	1.40	1.44
2	A	801	HEM	C4C-NC	2.23	1.43	1.39
2	B	801	HEM	FE-NC	2.22	2.02	1.95
6	A	806	MPD	C5-C4	2.18	1.60	1.51
2	A	801	HEM	C4D-C3D	-2.16	1.41	1.45
2	B	801	HEM	C4D-C3D	-2.15	1.41	1.45
2	B	801	HEM	C2A-C3A	-2.15	1.33	1.38
2	B	801	HEM	O2A-CGA	-2.14	1.23	1.30
2	B	801	HEM	C3C-C4C	2.11	1.49	1.46
2	A	801	HEM	O1A-CGA	2.04	1.28	1.22
2	A	801	HEM	C4A-NA	-2.02	1.35	1.39
2	B	801	HEM	O1D-CGD	2.02	1.28	1.22

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	806	MPD	O2-C2-CM	4.38	121.65	107.99
2	B	801	HEM	CBD-CAD-C3D	4.32	124.47	112.53
2	B	801	HEM	CAA-CBA-CGA	-4.08	102.86	113.67
2	B	801	HEM	CHD-C4C-NC	4.02	128.83	124.45
2	A	801	HEM	C4C-C3C-C2C	4.01	110.29	106.81
2	A	801	HEM	C3B-C2B-C1B	-4.00	103.40	106.41
2	A	801	HEM	CHB-C1B-NB	3.77	129.03	124.37
2	A	801	HEM	CMB-C2B-C1B	-3.74	119.19	125.03
2	B	801	HEM	O1D-CGD-CBD	-3.69	111.39	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	CAA-CBA-CGA	-3.48	104.44	113.67
6	A	806	MPD	O2-C2-C1	-3.46	97.21	107.99
2	A	801	HEM	CMB-C2B-C3B	3.36	136.56	128.43
2	A	801	HEM	CAA-C2A-C1A	3.36	131.50	124.94
2	B	801	HEM	CHC-C1C-NC	-3.29	120.87	124.45
2	A	801	HEM	C3D-C4D-ND	3.28	113.77	110.17
2	A	801	HEM	CBD-CAD-C3D	3.26	121.54	112.53
2	A	801	HEM	CAD-C3D-C4D	3.15	130.19	124.70
6	B	802	MPD	C1-C2-C3	3.10	123.59	110.20
2	A	801	HEM	O2D-CGD-CBD	3.00	123.49	114.00
2	A	801	HEM	C4D-C3D-C2D	-2.97	102.57	106.89
6	A	806	MPD	C1-C2-C3	2.84	122.45	110.20
2	A	801	HEM	CHC-C4B-NB	2.84	127.48	124.42
2	B	801	HEM	CAA-C2A-C1A	2.84	130.48	124.94
2	A	801	HEM	C4C-NC-C1C	2.82	110.42	105.82
2	A	801	HEM	C1B-NB-C4B	2.77	108.49	105.21
2	B	801	HEM	CMC-C2C-C1C	2.73	129.53	124.73
2	A	801	HEM	C4A-C3A-C2A	2.64	109.84	106.82
6	A	806	MPD	O4-C4-C3	-2.63	100.90	111.35
2	B	801	HEM	CHC-C4B-NB	2.62	127.25	124.42
2	A	801	HEM	C3C-C2C-C1C	-2.55	104.64	107.05
2	A	801	HEM	CHA-C4D-C3D	-2.53	120.56	125.23
2	A	801	HEM	CHB-C1B-C2B	-2.45	119.99	126.95
2	A	801	HEM	CMA-C3A-C4A	-2.43	121.72	125.42
6	A	805	MPD	O2-C2-C3	-2.41	100.26	109.27
2	A	801	HEM	CHD-C4C-C3C	2.37	129.20	125.21
2	B	801	HEM	CHA-C4D-C3D	-2.35	120.89	125.23
2	B	801	HEM	CMC-C2C-C3C	-2.33	122.79	128.43
6	A	806	MPD	O4-C4-C5	2.27	119.24	109.45
2	A	801	HEM	CBB-CAB-C3B	-2.27	116.18	127.53
6	B	802	MPD	O4-C4-C3	2.25	120.32	111.35
2	B	801	HEM	CHB-C4A-NA	2.19	127.84	123.86
2	A	801	HEM	O1D-CGD-CBD	-2.19	116.14	123.09
2	B	801	HEM	CMA-C3A-C4A	-2.18	122.09	125.42
2	B	801	HEM	C4C-NC-C1C	2.16	109.34	105.82
2	B	801	HEM	O1A-CGA-CBA	-2.16	116.25	123.09
6	A	806	MPD	CM-C2-C1	-2.15	105.81	110.63
6	A	805	MPD	O4-C4-C3	-2.09	103.04	111.35
6	A	805	MPD	C5-C4-C3	2.08	121.35	111.67
2	B	801	HEM	CMA-C3A-C2A	2.07	130.01	125.62
2	B	801	HEM	CHA-C1A-NA	2.02	127.52	123.86
2	A	801	HEM	CHD-C1D-ND	2.02	126.59	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	O2D-CGD-O1D	2.00	128.49	123.33

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	805	MPD	C2-C3-C4-C5
6	B	802	MPD	C2-C3-C4-O4
6	B	802	MPD	C2-C3-C4-C5
6	B	806	MPD	CM-C2-C3-C4
6	B	807	MPD	C1-C2-C3-C4
6	B	807	MPD	O2-C2-C3-C4
6	A	805	MPD	O2-C2-C3-C4
6	B	806	MPD	C1-C2-C3-C4
6	B	807	MPD	C2-C3-C4-C5
2	A	801	HEM	CAA-CBA-CGA-O2A
2	B	801	HEM	CAA-CBA-CGA-O1A
2	A	801	HEM	CAA-CBA-CGA-O1A
2	B	801	HEM	CAA-CBA-CGA-O2A
6	A	806	MPD	O2-C2-C3-C4
6	B	806	MPD	O2-C2-C3-C4
6	B	806	MPD	C2-C3-C4-O4
6	A	805	MPD	CM-C2-C3-C4
6	B	807	MPD	CM-C2-C3-C4

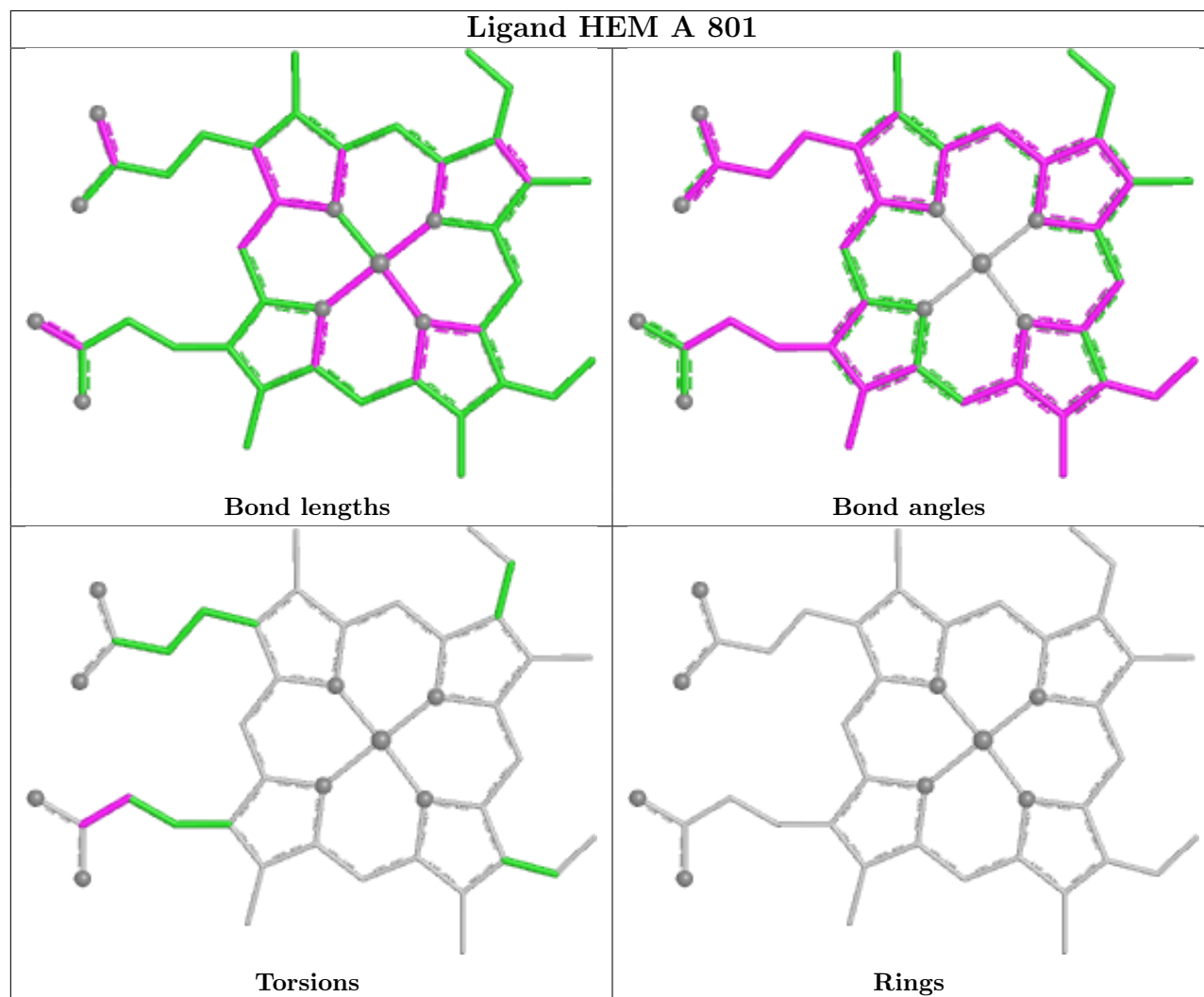
There are no ring outliers.

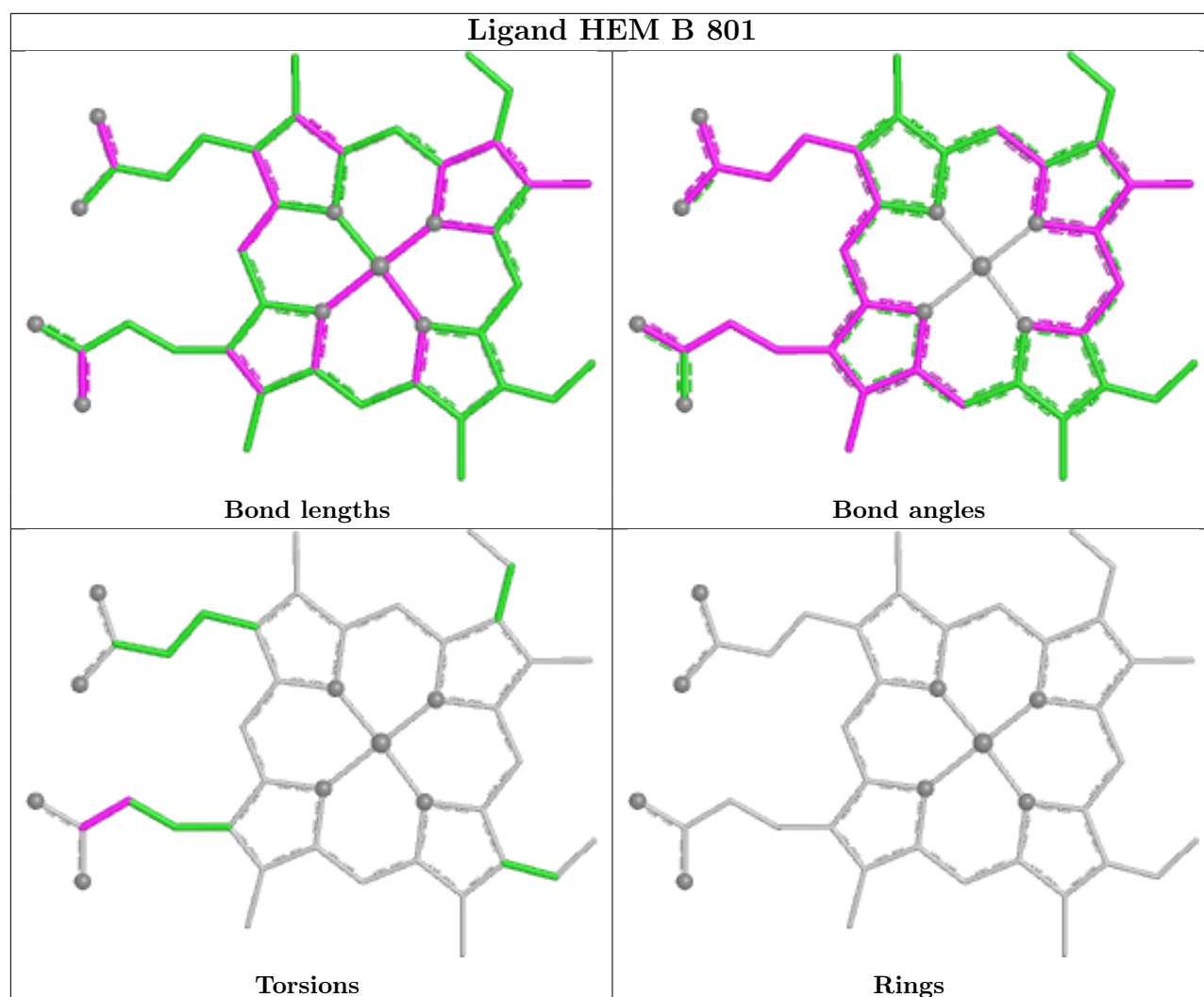
5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	807	MPD	1	0
6	B	802	MPD	6	0
6	B	806	MPD	2	0
6	A	806	MPD	1	0
6	A	805	MPD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	712/728 (97%)	-0.01	8 (1%) 78 82	13, 25, 44, 77	4 (0%)
1	B	712/728 (97%)	-0.08	12 (1%) 69 74	13, 24, 44, 87	8 (1%)
All	All	1424/1456 (97%)	-0.05	20 (1%) 73 79	13, 25, 44, 87	12 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	53	HIS	4.9
1	A	748	ALA	4.8
1	B	53	HIS	4.7
1	A	55	HIS	4.6
1	B	748	ALA	4.3
1	A	64	LYS	3.6
1	B	64	LYS	3.2
1	A	680	ALA	3.2
1	B	680	ALA	3.1
1	B	55	HIS	3.1
1	B	679	ALA	3.0
1	B	65	ASP	2.8
1	B	36	GLY	2.6
1	B	40	ARG	2.6
1	B	610	ARG	2.6
1	A	40	ARG	2.5
1	B	54	ARG	2.4
1	A	608	LYS	2.3
1	A	540	ARG	2.1
1	B	47	LEU	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
1	TOX	A	111[A]	16/17	0.97	0.06	19,21,26,27	2
1	TOX	A	111[B]	16/17	0.97	0.06	19,21,23,27	2
1	TOX	B	111[A]	16/17	0.97	0.06	15,19,26,26	1
1	TOX	B	111[B]	16/17	0.97	0.06	15,19,23,26	1

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

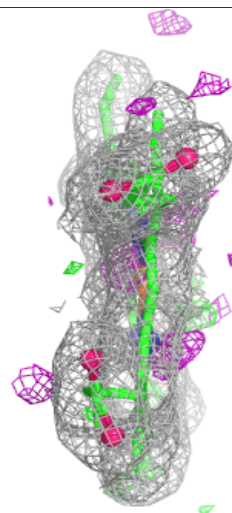
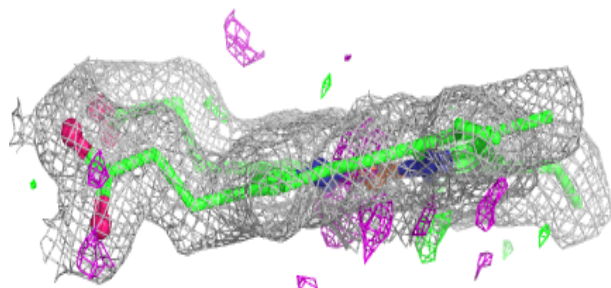
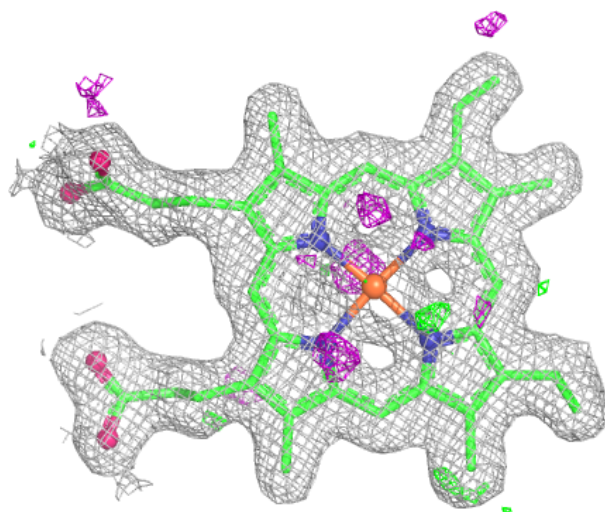
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MPD	B	807	8/8	0.81	0.27	54,59,66,66	0
6	MPD	A	806	8/8	0.84	0.17	47,53,55,56	0
6	MPD	A	805	8/8	0.85	0.19	45,50,57,57	0
6	MPD	B	806	8/8	0.86	0.14	41,46,48,50	0
6	MPD	B	802	8/8	0.87	0.14	40,46,48,48	0
5	OXY	B	805	2/2	0.89	0.26	40,40,40,42	0
5	OXY	A	804	2/2	0.93	0.21	37,37,37,40	0
4	CL	B	804	1/1	0.97	0.10	36,36,36,36	0
3	NA	B	803	1/1	0.98	0.05	22,22,22,22	0
4	CL	A	803	1/1	0.98	0.06	40,40,40,40	0
2	HEM	A	801	43/43	0.98	0.07	16,20,22,23	0
2	HEM	B	801	43/43	0.98	0.06	17,20,22,23	0
3	NA	A	802	1/1	0.98	0.06	22,22,22,22	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.

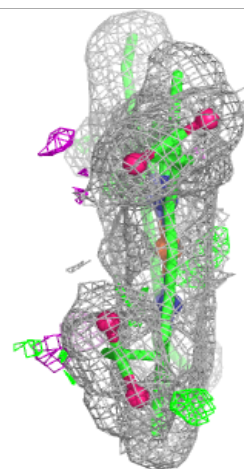
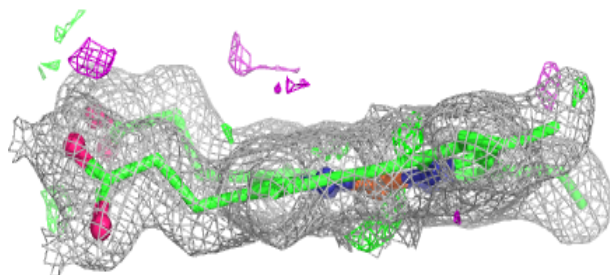
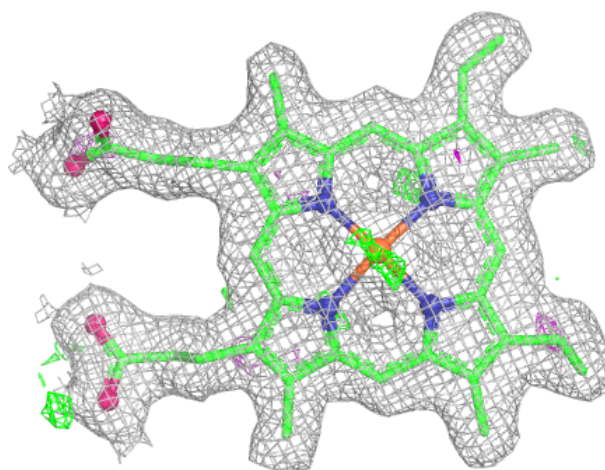
Electron density around HEM A 801:

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



Electron density around HEM B 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.