



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2017 – 08:46 PM EDT

PDB ID : 5KSK
Title : Crystal structure of the catalase-peroxidase from *B. pseudomallei* treated with acetate
Authors : Loewen, P.C.
Deposited on : unknown
Resolution : 1.69 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

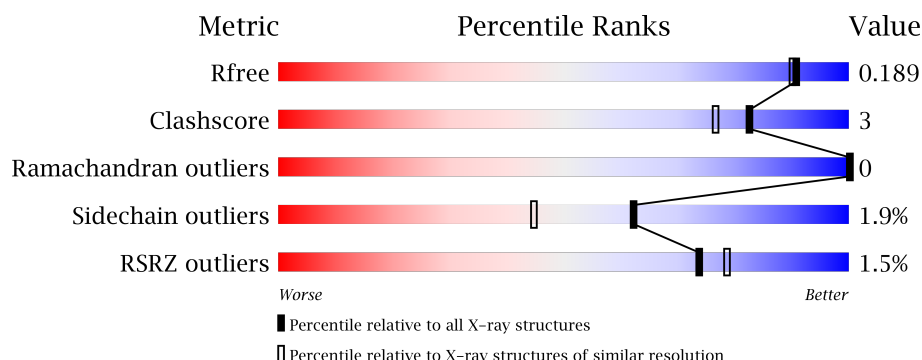
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.69 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}	100719	3453 (1.70-1.70)
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)
RSRZ outliers	101464	3491 (1.70-1.70)

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. 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>2%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>..</div> </div> </div>
1	B	728	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>10%</div> <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
6	MPD	A	806	-	-	-	X
6	MPD	B	805	-	-	X	X
6	MPD	B	806	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12836 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	6	0
			5546	3503	989	1040	14			
1	B	713	Total	C	N	O	S	0	9	0
			5548	3506	987	1041	14			

- 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		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

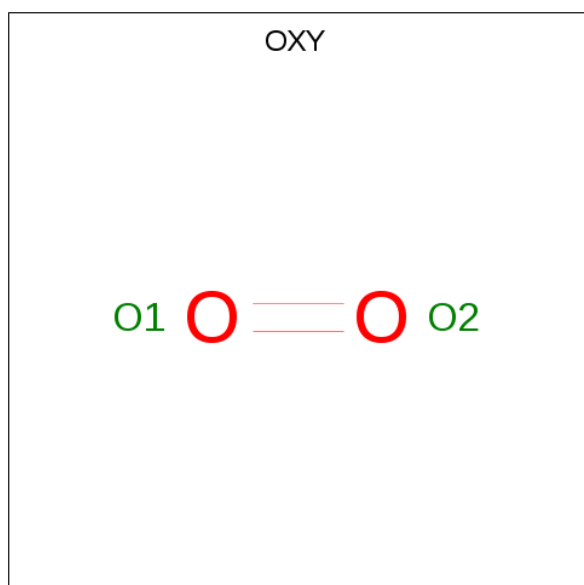
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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	B	1	Total O 2 2	0	0

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



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

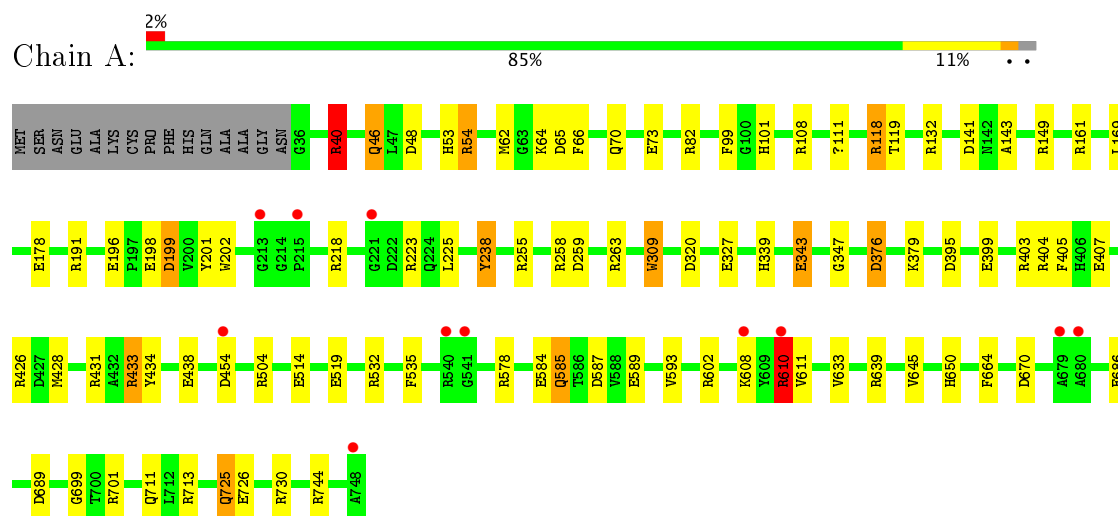
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	821	Total O 821 821	0	0
7	B	787	Total O 787 787	0	0

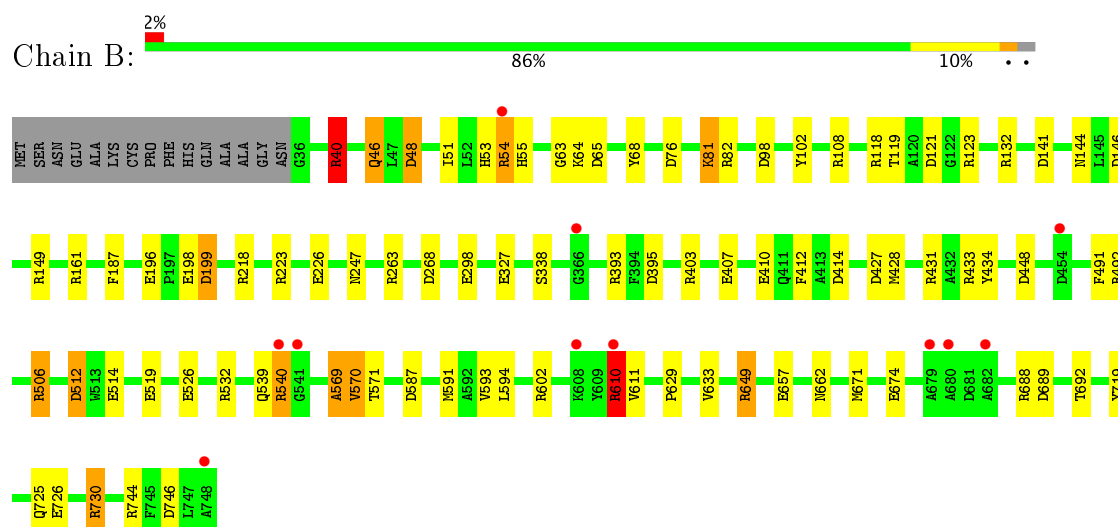
3 Residue-property plots

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 ($RSRZ > 2$). 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: Catalase-peroxidase



• Molecule 1: Catalase-peroxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.70 Å 115.48 Å 174.97 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.39 – 1.69 48.39 – 1.69	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.39-1.69) 99.2 (48.39-1.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 1.69 Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.152 , 0.180 0.164 , 0.189	Depositor DCC
R_{free} test set	11161 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12836	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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: TOX, OXY, CL, NA, MPD, 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	1.50	34/5688 (0.6%)	1.30	50/7729 (0.6%)
1	B	1.46	30/5696 (0.5%)	1.34	60/7741 (0.8%)
All	All	1.48	64/11384 (0.6%)	1.32	110/15470 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
All	All	0	4

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	726	GLU	CD-OE1	10.50	1.37	1.25
1	B	512	ASP	CG-OD2	9.95	1.48	1.25
1	A	343	GLU	CD-OE2	9.81	1.36	1.25
1	B	512	ASP	CB-CG	9.29	1.71	1.51
1	A	407	GLU	CG-CD	8.10	1.64	1.51
1	A	407	GLU	CD-OE1	7.91	1.34	1.25
1	B	746	ASP	CB-CG	7.91	1.68	1.51
1	A	725	GLN	CG-CD	7.69	1.68	1.51
1	A	633	VAL	CB-CG1	-7.51	1.37	1.52
1	A	584	GLU	CG-CD	7.45	1.63	1.51
1	A	726	GLU	CG-CD	7.24	1.62	1.51
1	A	196	GLU	CG-CD	7.17	1.62	1.51
1	A	589	GLU	CD-OE1	7.13	1.33	1.25
1	B	526	GLU	CD-OE1	7.09	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	540	ARG	C-O	7.07	1.36	1.23
1	B	81	LYS	CE-NZ	7.05	1.66	1.49
1	B	410	GLU	CG-CD	7.04	1.62	1.51
1	A	70	GLN	CG-CD	6.85	1.66	1.51
1	A	686	GLU	CG-CD	6.80	1.62	1.51
1	B	198	GLU	CD-OE2	6.65	1.32	1.25
1	B	327	GLU	CD-OE2	6.63	1.32	1.25
1	A	201	TYR	CG-CD2	-6.61	1.30	1.39
1	B	671	MET	CG-SD	-6.57	1.64	1.81
1	B	81	LYS	CD-CE	6.38	1.67	1.51
1	B	102	TYR	CE1-CZ	-6.22	1.30	1.38
1	B	434	TYR	CE2-CZ	-6.11	1.30	1.38
1	B	226	GLU	CD-OE2	-5.91	1.19	1.25
1	A	532	ARG	NE-CZ	-5.90	1.25	1.33
1	B	196	GLU	CB-CG	-5.87	1.41	1.52
1	B	602	ARG	CZ-NH2	-5.86	1.25	1.33
1	A	535	PHE	CG-CD1	-5.84	1.29	1.38
1	B	196	GLU	CG-CD	5.79	1.60	1.51
1	B	407	GLU	CD-OE1	-5.68	1.19	1.25
1	A	202	TRP	CG-CD1	-5.64	1.28	1.36
1	A	82	ARG	CZ-NH2	-5.64	1.25	1.33
1	B	726	GLU	CG-CD	5.62	1.60	1.51
1	B	298	GLU	CD-OE2	5.59	1.31	1.25
1	A	584	GLU	CD-OE2	5.59	1.31	1.25
1	B	82	ARG	CZ-NH2	-5.51	1.25	1.33
1	A	585	GLN	CD-OE1	5.49	1.36	1.24
1	A	73	GLU	CG-CD	5.48	1.60	1.51
1	B	657	GLU	CG-CD	5.45	1.60	1.51
1	A	454	ASP	CB-CG	5.43	1.63	1.51
1	A	434	TYR	CE2-CZ	-5.42	1.31	1.38
1	A	584	GLU	CD-OE1	5.34	1.31	1.25
1	A	711	GLN	CD-NE2	-5.31	1.19	1.32
1	B	526	GLU	CG-CD	5.29	1.59	1.51
1	A	178	GLU	CG-CD	5.26	1.59	1.51
1	A	327	GLU	CG-CD	5.23	1.59	1.51
1	A	438	GLU	CD-OE1	-5.20	1.20	1.25
1	B	338	SER	CB-OG	-5.19	1.35	1.42
1	B	247	ASN	CB-CG	5.17	1.62	1.51
1	A	347	GLY	N-CA	5.13	1.53	1.46
1	A	699	GLY	N-CA	5.11	1.53	1.46
1	A	62	MET	C-N	-5.10	1.23	1.33
1	A	198	GLU	CD-OE2	5.09	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	399	GLU	CD-OE2	5.08	1.31	1.25
1	A	309	TRP	CZ3-CH2	-5.08	1.31	1.40
1	B	448	ASP	N-CA	5.08	1.56	1.46
1	B	674	GLU	CG-CD	5.05	1.59	1.51
1	B	68	TYR	CG-CD2	-5.02	1.32	1.39
1	A	514	GLU	CD-OE1	-5.01	1.20	1.25
1	A	519	GLU	CD-OE1	5.01	1.31	1.25
1	B	63	GLY	N-CA	5.00	1.53	1.46

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	512	ASP	CB-CG-OD1	-15.22	104.60	118.30
1	B	149	ARG	NE-CZ-NH2	-10.94	114.83	120.30
1	A	149	ARG	NE-CZ-NH1	10.52	125.56	120.30
1	B	268	ASP	CB-CG-OD1	10.33	127.60	118.30
1	A	40	ARG	NE-CZ-NH1	10.24	125.42	120.30
1	B	433	ARG	NE-CZ-NH2	-10.14	115.23	120.30
1	A	82	ARG	NE-CZ-NH1	9.95	125.27	120.30
1	A	701	ARG	NE-CZ-NH1	9.39	124.99	120.30
1	A	713	ARG	NE-CZ-NH2	-9.27	115.67	120.30
1	B	403	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	A	82	ARG	NE-CZ-NH2	-9.05	115.78	120.30
1	B	688	ARG	NE-CZ-NH1	9.01	124.81	120.30
1	B	730	ARG	NE-CZ-NH1	8.91	124.75	120.30
1	B	132	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	B	82	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	B	123	ARG	NE-CZ-NH2	-8.71	115.95	120.30
1	B	40	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	A	532	ARG	NE-CZ-NH2	-8.53	116.04	120.30
1	A	730	ARG	NE-CZ-NH1	8.41	124.51	120.30
1	A	713	ARG	NE-CZ-NH1	8.41	124.51	120.30
1	A	263	ARG	NE-CZ-NH2	-8.35	116.13	120.30
1	B	492	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	B	82	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	B	730	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	B	434	TYR	CB-CG-CD1	8.22	125.93	121.00
1	A	578	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	A	118	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	A	587	ASP	CB-CG-OD1	7.69	125.22	118.30
1	B	263	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	A	744	ARG	NE-CZ-NH2	-7.58	116.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	512	ASP	CB-CG-OD2	7.57	125.12	118.30
1	B	123	ARG	NE-CZ-NH1	7.55	124.07	120.30
1	B	108	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	B	433	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	B	587	ASP	CB-CG-OD1	7.11	124.70	118.30
1	A	633	VAL	CG1-CB-CG2	-7.07	99.58	110.90
1	B	393	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	B	199	ASP	CB-CG-OD1	-6.95	112.05	118.30
1	B	514	GLU	OE1-CD-OE2	-6.95	114.96	123.30
1	B	570	VAL	CG1-CB-CG2	-6.93	99.81	110.90
1	A	434	TYR	CB-CG-CD1	6.92	125.15	121.00
1	A	431	ARG	NE-CZ-NH2	6.76	123.68	120.30
1	A	46	GLN	CA-CB-CG	6.70	128.13	113.40
1	B	403	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	639	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	403	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	A	132	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	B	81	LYS	CD-CE-NZ	6.50	126.64	111.70
1	B	161	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	A	433	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	B	744	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	66	PHE	CB-CG-CD1	-6.44	116.29	120.80
1	B	414	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	B	649[A]	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	B	649[B]	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	B	427	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	B	98	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	B	610	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	B	689	ASP	CB-CG-OD1	6.13	123.81	118.30
1	A	730	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	A	584	GLU	OE1-CD-OE2	-6.05	116.04	123.30
1	A	395	ASP	CB-CG-OD1	6.05	123.74	118.30
1	A	670	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	B	602	ARG	NE-CZ-NH1	-5.89	117.35	120.30
1	B	48	ASP	CB-CG-OD2	5.86	123.57	118.30
1	B	65	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	B	448	ASP	CB-CG-OD1	5.74	123.47	118.30
1	B	76	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	B	68	TYR	CB-CG-CD1	-5.70	117.58	121.00
1	B	492	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	40	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	664	PHE	CB-CG-CD1	-5.63	116.86	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	ILE	CG1-CB-CG2	-5.56	99.16	111.40
1	B	491	PHE	CG-CD2-CE2	-5.54	114.71	120.80
1	B	532	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	A	161	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	169	LEU	CB-CG-CD2	5.50	120.35	111.00
1	A	689	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	238	TYR	CB-CG-CD2	5.43	124.25	121.00
1	A	701	ARG	NH1-CZ-NH2	-5.41	113.45	119.40
1	B	428	MET	CA-CB-CG	-5.40	104.12	113.30
1	A	405	PHE	CB-CG-CD2	-5.39	117.02	120.80
1	B	40	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	A	320	ASP	CB-CG-OD1	-5.38	113.46	118.30
1	B	149	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	395	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	610	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	121	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	A	404	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	407	GLU	CG-CD-OE1	5.28	128.87	118.30
1	B	726	GLU	CG-CD-OE1	5.26	128.83	118.30
1	B	506	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	376	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	A	255[A]	ARG	CB-CG-CD	5.19	125.09	111.60
1	A	255[B]	ARG	CB-CG-CD	5.19	125.09	111.60
1	B	54	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	65	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	B	46	GLN	CB-CG-CD	5.17	125.04	111.60
1	B	412	PHE	CB-CG-CD2	-5.17	117.18	120.80
1	A	258	ARG	NE-CZ-NH2	5.17	122.88	120.30
1	A	225	LEU	CB-CG-CD2	-5.16	102.22	111.00
1	B	218	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	744	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	218	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	A	259	ASP	CB-CG-OD2	-5.05	113.76	118.30
1	A	191	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	540	ARG	N-CA-CB	5.04	119.67	110.60
1	A	108	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	B	187	PHE	CB-CG-CD2	5.02	124.31	120.80
1	B	726	GLU	CG-CD-OE2	-5.01	108.28	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	ASP	Mainchain
1	B	199	ASP	Mainchain
1	B	539	GLN	Peptide
1	B	569	ALA	Mainchain

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	5546	0	5370	22	0
1	B	5548	0	5378	32	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	24	0	42	3	0
6	B	16	0	28	10	0
7	A	821	0	0	11	0
7	B	787	0	0	17	0
All	All	12836	0	10878	64	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 (64) 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:506:ARG:HE	6:B:805:MPD:H12	1.31	0.94
1:A:119[B]:THR:HG21	7:A:1049:HOH:O	1.72	0.87
1:A:426[A]:ARG:NE	7:A:905:HOH:O	1.67	0.87
6:B:805:MPD:H51	7:B:1353:HOH:O	1.81	0.79
6:B:805:MPD:H13	7:B:1543:HOH:O	1.85	0.75
1:B:512:ASP:OD1	7:B:903:HOH:O	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:HIS:HD2	7:B:1386:HOH:O	1.72	0.72
6:B:806:MPD:C1	6:B:806:MPD:O4	2.40	0.70
1:B:431:ARG:HD2	7:B:1468:HOH:O	1.92	0.68
1:B:519:GLU:OE1	7:B:904:HOH:O	2.11	0.68
1:B:54:ARG:O	7:B:906:HOH:O	2.12	0.68
1:B:569:ALA:O	1:B:570:VAL:HG23	1.96	0.66
1:A:53:HIS:NE2	7:A:908:HOH:O	2.30	0.64
6:A:806:MPD:HO4	6:A:806:MPD:HO2	1.45	0.63
1:B:81:LYS:CE	7:B:1097:HOH:O	2.46	0.62
1:B:431:ARG:CD	7:B:1468:HOH:O	2.46	0.61
6:A:805:MPD:H53	6:A:805:MPD:H11	1.81	0.61
1:B:81:LYS:HD3	7:B:1097:HOH:O	2.00	0.61
1:A:99:PHE:O	1:A:101[B]:HIS:HD2	1.86	0.59
1:B:81:LYS:CD	7:B:1097:HOH:O	2.49	0.59
6:A:806:MPD:O2	6:A:806:MPD:O4	2.14	0.58
1:B:506:ARG:HE	6:B:805:MPD:C1	2.10	0.58
1:B:506:ARG:NE	6:B:805:MPD:H12	2.12	0.58
1:B:53:HIS:CD2	7:B:1347:HOH:O	2.57	0.57
1:B:662:ASN:H	1:B:725:GLN:HE22	1.52	0.56
1:B:53:HIS:HD2	7:B:1347:HOH:O	1.87	0.56
1:B:591:MET:SD	1:B:594:LEU:HD12	2.47	0.55
1:A:119[B]:THR:HG23	1:A:593:VAL:HG11	1.87	0.55
1:A:426[A]:ARG:CG	7:A:905:HOH:O	2.54	0.55
6:B:805:MPD:C1	6:B:805:MPD:H52	2.37	0.54
1:B:119[B]:THR:CG2	7:B:1119:HOH:O	2.54	0.54
1:A:343:GLU:OE1	7:A:906:HOH:O	2.19	0.52
1:B:610:ARG:HD2	1:B:611:VAL:HG23	1.91	0.51
1:A:376:ASP:OD2	1:A:379:LYS:HE3	2.11	0.50
1:B:569:ALA:O	1:B:570:VAL:CG2	2.59	0.50
1:A:585:GLN:NE2	7:A:921:HOH:O	2.45	0.50
1:A:593:VAL:HG13	7:A:912:HOH:O	2.12	0.49
1:A:610:ARG:HD2	1:A:611:VAL:HG23	1.95	0.49
1:A:426[A]:ARG:HG2	7:A:905:HOH:O	2.12	0.49
1:A:504:ARG:HD2	7:A:951:HOH:O	2.12	0.48
1:B:119[B]:THR:HG22	7:B:1119:HOH:O	2.13	0.48
1:B:633[A]:VAL:HG22	1:B:719:TYR:CZ	2.49	0.48
1:B:629:PRO:O	1:B:633[A]:VAL:HG23	2.13	0.47
1:B:119[B]:THR:HG22	1:B:593:VAL:HG21	1.96	0.47
1:A:650:HIS:HE1	7:A:1555:HOH:O	1.96	0.47
1:A:54:ARG:HG3	1:A:199:ASP:OD2	2.16	0.46
1:B:40:ARG:NH2	1:B:48:ASP:HB2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:ASP:HB2	7:B:1447:HOH:O	2.17	0.44
1:A:40:ARG:NH2	1:A:48:ASP:HB2	2.32	0.44
1:B:633[A]:VAL:HG22	1:B:719:TYR:CE2	2.52	0.44
6:B:806:MPD:O4	6:B:806:MPD:H12	2.16	0.43
1:B:144:ASN:HA	1:B:146:ASP:OD1	2.18	0.43
1:B:119[B]:THR:HG23	7:B:1119:HOH:O	2.19	0.43
6:B:806:MPD:H11	6:B:806:MPD:O4	2.16	0.43
1:A:339:HIS:HB2	7:A:1372:HOH:O	2.19	0.42
1:A:602:ARG:HB3	1:A:645:VAL:HG23	2.01	0.42
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	3.03	0.42
6:B:805:MPD:H12	6:B:805:MPD:H52	2.00	0.42
1:A:111:TOX:H9	1:A:238:TYR:OH	2.19	0.42
1:A:143:ALA:HA	1:A:309:TRP:CH2	2.55	0.42
1:A:428:MET:O	1:A:433:ARG:HD3	2.20	0.41
1:A:376:ASP:OD2	1:A:379:LYS:CE	2.68	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	716/728 (98%)	707 (99%)	9 (1%)	0	100	100
1	B	718/728 (99%)	710 (99%)	8 (1%)	0	100	100
All	All	1434/1456 (98%)	1417 (99%)	17 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	555/560 (99%)	545 (98%)	10 (2%)	64	47
1	B	557/560 (100%)	545 (98%)	12 (2%)	57	38
All	All	1112/1120 (99%)	1090 (98%)	22 (2%)	62	42

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	46	GLN
1	A	54	ARG
1	A	64	LYS
1	A	118	ARG
1	A	141	ASP
1	A	223	ARG
1	A	608	LYS
1	A	610	ARG
1	A	725	GLN
1	B	40	ARG
1	B	46	GLN
1	B	64	LYS
1	B	118	ARG
1	B	141	ASP
1	B	223	ARG
1	B	540	ARG
1	B	571	THR
1	B	610	ARG
1	B	649[A]	ARG
1	B	649[B]	ARG
1	B	730	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	247	ASN
1	B	53	HIS
1	B	55	HIS
1	B	227	ASN

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Mol	Chain	Res	Type
1	B	647	GLN
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 ⓘ

3 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	1	12,17,18	2.88	6 (50%)	11,23,25	1.91	1 (9%)
1	TOX	B	111[A]	2	12,17,18	2.41	6 (50%)	11,23,25	2.53	4 (36%)
1	TOX	B	111[B]	-	12,17,18	2.41	6 (50%)	11,23,25	2.53	4 (36%)

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	1	-	0/3/8/10	0/2/2/2
1	TOX	B	111[A]	2	-	0/3/8/10	0/2/2/2
1	TOX	B	111[B]	-	-	0/3/8/10	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	TOX	CD1-NE1	-7.47	1.32	1.39
1	B	111[B]	TOX	CD1-NE1	-4.12	1.35	1.39
1	B	111[A]	TOX	CD1-NE1	-4.12	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111[B]	TOX	CZ2-CE2	-2.65	1.35	1.41
1	B	111[A]	TOX	CZ2-CE2	-2.65	1.35	1.41
1	B	111[B]	TOX	CB-CA	-2.64	1.47	1.53
1	B	111[A]	TOX	CB-CA	-2.64	1.47	1.53
1	B	111[B]	TOX	CE3-CD2	-2.37	1.37	1.42
1	B	111[A]	TOX	CE3-CD2	-2.37	1.37	1.42
1	A	111	TOX	CH2-CZ2	2.11	1.41	1.36
1	A	111	TOX	O1-NE1	2.11	1.42	1.38
1	B	111[B]	TOX	CZ3-CE3	2.35	1.42	1.36
1	B	111[A]	TOX	CZ3-CE3	2.35	1.42	1.36
1	A	111	TOX	O-C	2.52	1.30	1.19
1	A	111	TOX	CZ3-CH2	2.63	1.44	1.38
1	A	111	TOX	CA-C	4.11	1.55	1.50
1	B	111[B]	TOX	O-C	4.45	1.38	1.19
1	B	111[A]	TOX	O-C	4.45	1.38	1.19

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	TOX	CB-CG-CD1	-5.05	121.73	127.97
1	B	111[B]	TOX	CZ3-CH2-CZ2	-4.85	113.53	120.45
1	B	111[A]	TOX	CZ3-CH2-CZ2	-4.85	113.53	120.45
1	B	111[B]	TOX	CZ2-CE2-CD2	-3.84	115.71	120.94
1	B	111[A]	TOX	CZ2-CE2-CD2	-3.84	115.71	120.94
1	B	111[B]	TOX	CZ3-CE3-CD2	-2.96	116.64	120.88
1	B	111[A]	TOX	CZ3-CE3-CD2	-2.96	116.64	120.88
1	B	111[B]	TOX	CH2-CZ2-CE2	3.98	127.33	119.33
1	B	111[A]	TOX	CH2-CZ2-CE2	3.98	127.33	119.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	111	TOX	1	0

5.5 Carbohydrates ⓘ

There are no carbohydrates 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
2	HEM	A	801	1	28,50,50	2.17	6 (21%)	17,82,82	2.41	7 (41%)
5	OXY	A	804	-	1,1,1	0.16	0	0,0,0	0.00	-
6	MPD	A	805	-	7,7,7	0.56	0	9,10,10	1.40	1 (11%)
6	MPD	A	806	-	7,7,7	0.54	0	9,10,10	1.48	2 (22%)
6	MPD	A	807	-	7,7,7	0.73	0	9,10,10	1.25	1 (11%)
2	HEM	B	801	1	28,50,50	2.50	11 (39%)	17,82,82	2.47	7 (41%)
5	OXY	B	804	-	1,1,1	0.29	0	0,0,0	0.00	-
6	MPD	B	805	-	7,7,7	1.19	1 (14%)	9,10,10	0.93	0
6	MPD	B	806	-	7,7,7	0.63	0	9,10,10	1.89	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
2	HEM	A	801	1	-	0/6/54/54	0/0/8/8
5	OXY	A	804	-	-	0/0/0/0	0/0/0/0
6	MPD	A	805	-	-	0/5/5/5	0/0/0/0
6	MPD	A	806	-	-	0/5/5/5	0/0/0/0
6	MPD	A	807	-	-	0/5/5/5	0/0/0/0
2	HEM	B	801	1	-	0/6/54/54	0/0/8/8
5	OXY	B	804	-	-	0/0/0/0	0/0/0/0
6	MPD	B	805	-	-	0/5/5/5	0/0/0/0
6	MPD	B	806	-	-	0/5/5/5	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C1B-NB	-7.52	1.27	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C1C-NC	-5.50	1.30	1.36
2	B	801	HEM	C1B-NB	-5.11	1.30	1.36
2	B	801	HEM	C3C-C2C	-3.32	1.36	1.40
2	B	801	HEM	CMD-C2D	-3.22	1.45	1.51
2	B	801	HEM	C4A-NA	-2.91	1.29	1.36
2	A	801	HEM	C1A-CHA	-2.58	1.33	1.40
2	B	801	HEM	CAD-C3D	-2.38	1.48	1.52
2	B	801	HEM	C1D-ND	2.03	1.40	1.36
2	A	801	HEM	C1C-NC	2.08	1.39	1.36
2	B	801	HEM	C4B-CHC	2.28	1.46	1.40
6	B	805	MPD	C3-C2	2.32	1.60	1.53
2	A	801	HEM	CMA-C3A	2.37	1.56	1.51
2	B	801	HEM	C4B-NB	2.51	1.41	1.36
2	A	801	HEM	C4D-ND	2.95	1.40	1.36
2	B	801	HEM	C1A-NA	3.37	1.43	1.36
2	A	801	HEM	C1D-ND	4.63	1.46	1.36
2	B	801	HEM	C4C-NC	6.06	1.43	1.36

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	CMA-C3A-C4A	-5.07	120.67	128.46
2	A	801	HEM	CAA-CBA-CGA	-4.63	104.75	112.66
6	B	806	MPD	CM-C2-C1	-3.15	103.39	110.42
2	B	801	HEM	CAA-C2A-C3A	-3.02	120.39	129.00
2	A	801	HEM	C3C-C4C-NC	-2.76	105.74	110.94
6	B	806	MPD	O2-C2-C3	-2.71	99.14	109.88
2	A	801	HEM	CMD-C2D-C1D	-2.56	124.53	128.46
6	A	807	MPD	O2-C2-CM	-2.55	99.17	108.00
6	B	806	MPD	O4-C4-C5	-2.36	98.62	109.46
6	A	805	MPD	CM-C2-C1	-2.35	105.18	110.42
6	A	806	MPD	CM-C2-C1	-2.17	105.59	110.42
2	B	801	HEM	CMC-C2C-C3C	2.08	128.76	124.89
2	A	801	HEM	CMD-C2D-C3D	2.47	129.59	124.94
6	B	806	MPD	C1-C2-C3	2.50	122.51	110.08
2	B	801	HEM	C4C-C3C-C2C	2.57	108.69	106.90
2	B	801	HEM	CBD-CAD-C3D	2.58	117.39	112.47
6	A	806	MPD	O2-C2-CM	2.76	117.58	108.00
2	A	801	HEM	CBD-CAD-C3D	3.55	119.24	112.47
2	A	801	HEM	CMB-C2B-C3B	3.71	131.77	124.89
2	B	801	HEM	CMA-C3A-C2A	3.93	132.35	124.94
2	A	801	HEM	CAD-CBD-CGD	3.99	119.48	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	CAD-CBD-CGD	4.98	121.17	112.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	805	MPD	1	0
6	A	806	MPD	2	0
6	B	805	MPD	7	0
6	B	806	MPD	3	0

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%)	-0.33	11 (1%) 74 78	15, 23, 41, 81	0
1	B	712/728 (97%)	-0.38	11 (1%) 74 78	15, 22, 41, 91	0
All	All	1424/1456 (97%)	-0.36	22 (1%) 74 78	15, 22, 41, 91	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	748	ALA	5.8
1	A	748	ALA	5.6
1	B	610	ARG	4.4
1	B	679	ALA	4.4
1	B	541	GLY	4.0
1	A	540	ARG	3.9
1	A	541	GLY	3.9
1	A	610	ARG	3.6
1	B	540	ARG	3.2
1	B	680	ALA	3.1
1	A	679	ALA	3.1
1	A	454	ASP	2.9
1	A	608	LYS	2.8
1	A	680	ALA	2.6
1	B	608	LYS	2.5
1	A	213	GLY	2.4
1	A	215	PRO	2.3
1	B	366	GLY	2.2
1	A	221	GLY	2.2
1	B	682	ALA	2.2
1	B	454	ASP	2.1
1	B	54	ARG	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
1	TOX	A	111	16/17	0.97	0.10	-	14,16,25,26	2
1	TOX	B	111[B]	16/17	0.98	0.13	-	15,16,18,22	3
1	TOX	B	111[A]	16/17	0.98	0.13	-	15,16,21,22	3

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
6	MPD	B	805	8/8	0.89	0.19	16.19	32,44,48,48	0
6	MPD	A	806	8/8	0.89	0.16	8.49	51,59,73,75	0
6	MPD	B	806	8/8	0.86	0.17	4.06	56,66,71,75	0
2	HEM	B	801	43/43	0.98	0.10	0.45	15,16,19,24	0
2	HEM	A	801	43/43	0.98	0.08	0.05	16,19,22,23	0
3	NA	B	802	1/1	0.97	0.06	-0.41	20,20,20,20	0
3	NA	A	802	1/1	0.99	0.08	-0.56	19,19,19,19	0
4	CL	B	803	1/1	0.99	0.06	-1.43	32,32,32,32	0
4	CL	A	803	1/1	0.99	0.04	-3.58	30,30,30,30	0
5	OXY	B	804	2/2	0.93	0.11	-	35,35,35,36	0
6	MPD	A	805	8/8	0.92	0.13	-	44,50,61,63	0
5	OXY	A	804	2/2	0.90	0.17	-	42,42,42,43	0
6	MPD	A	807	8/8	0.70	0.27	-	60,68,73,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.