



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2017 – 04:47 AM EDT

PDB ID : 5V53
Title : Crystal structure of the D141A/Q233E/N240D variant of catalase-peroxidase from *B. pseudomallei* with acetate bound
Authors : Loewen, P.C.
Deposited on : unknown
Resolution : 1.70 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

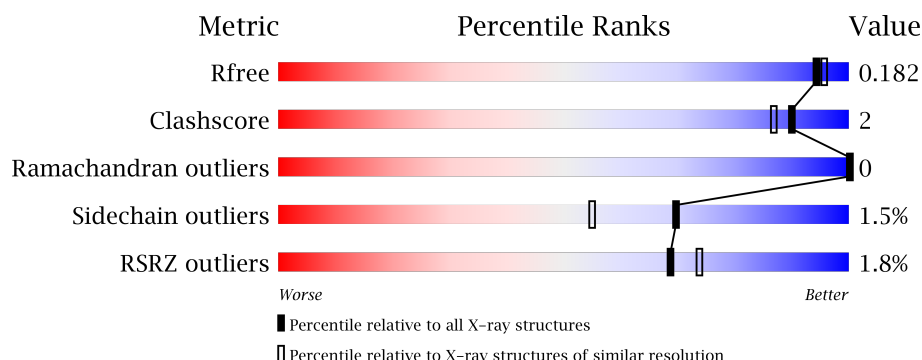
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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>86%</div> <div>11%</div> <div>..</div> </div> </div>
1	B	728	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>12%</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
5	OXY	A	804	-	-	X	-
5	OXY	B	804	-	-	X	-
6	ACT	A	805	-	-	X	X
6	ACT	B	805	-	-	X	-
8	MPD	A	807	-	-	-	X
8	MPD	B	807	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 12701 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.

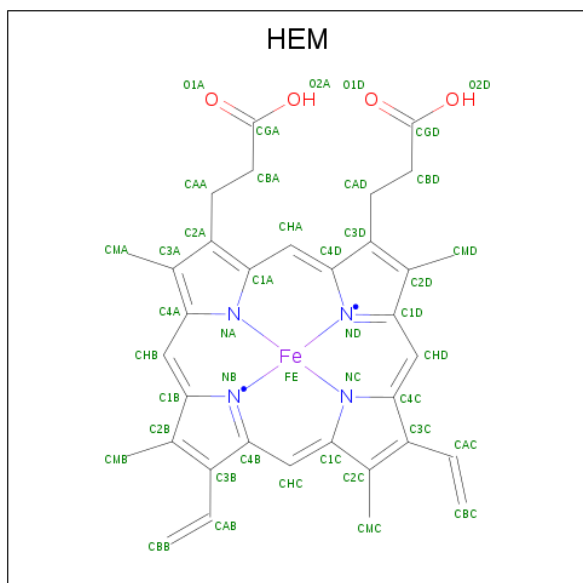
- Molecule 1 is a protein called Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total	C	N	O	S	0	6	0
			5550	3505	989	1042	14			
1	B	713	Total	C	N	O	S	0	6	0
			5542	3502	986	1040	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	ALA	ASP	engineered mutation	UNP Q3JNW6
A	233	GLU	GLN	engineered mutation	UNP Q3JNW6
A	240	ASP	ASN	engineered mutation	UNP Q3JNW6
B	141	ALA	ASP	engineered mutation	UNP Q3JNW6
B	233	GLU	GLN	engineered mutation	UNP Q3JNW6
B	240	ASP	ASN	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		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

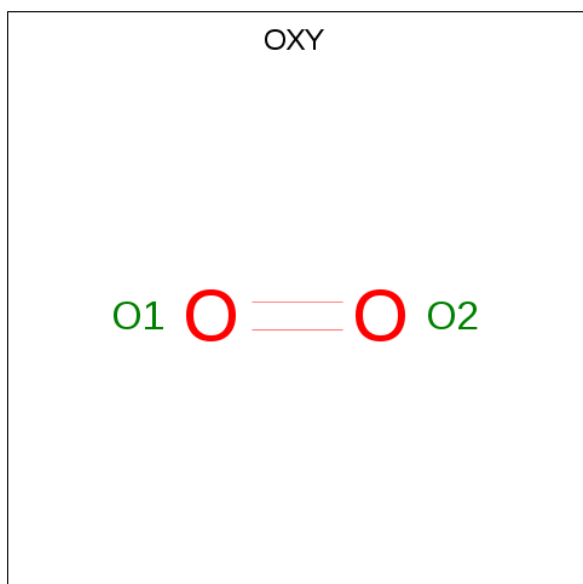
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

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

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

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



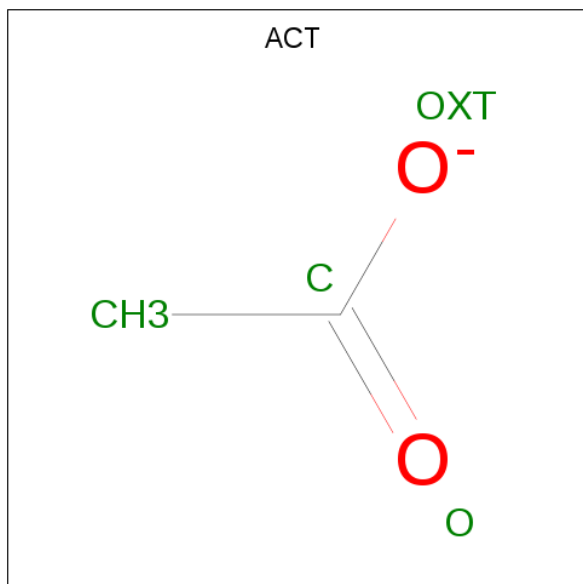
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			2	2		

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

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



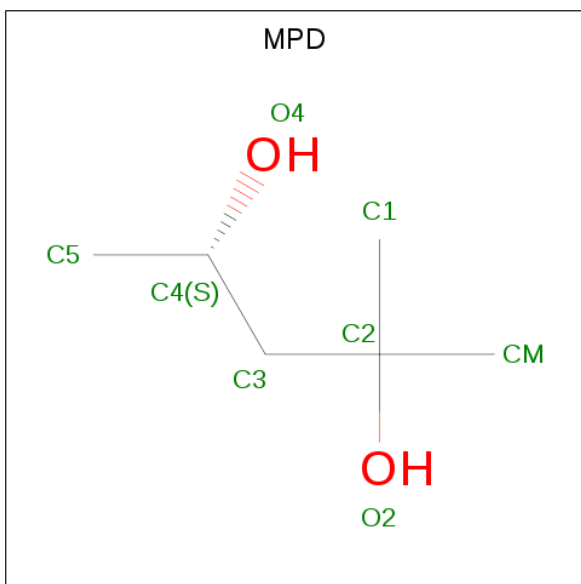
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is PHOSPHATE ION (three-letter code: PO₄) (formula: O_4P).



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

- Molecule 8 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



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

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

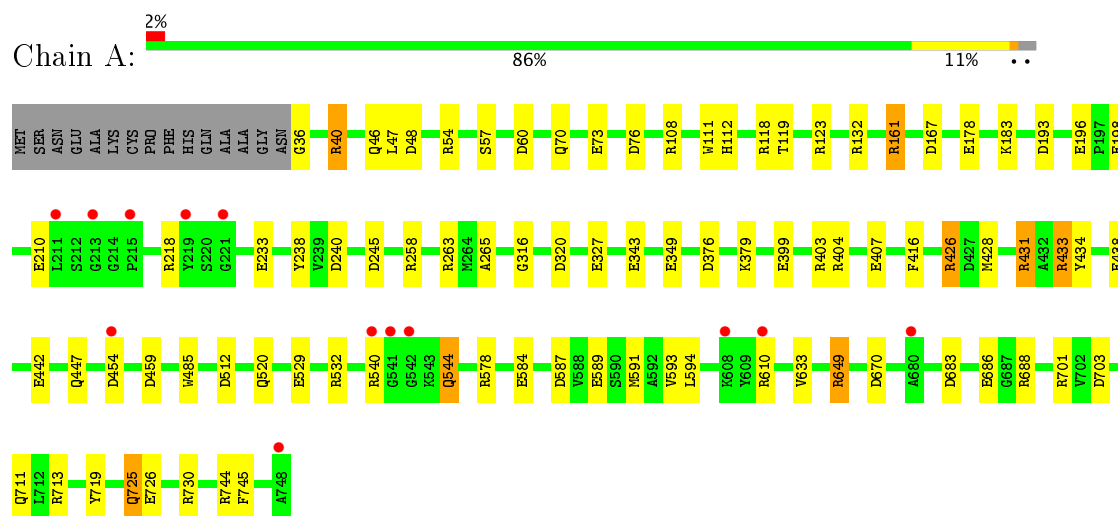
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	738	Total	O	0	0
			738	738		
9	B	727	Total	O	0	0
			727	727		

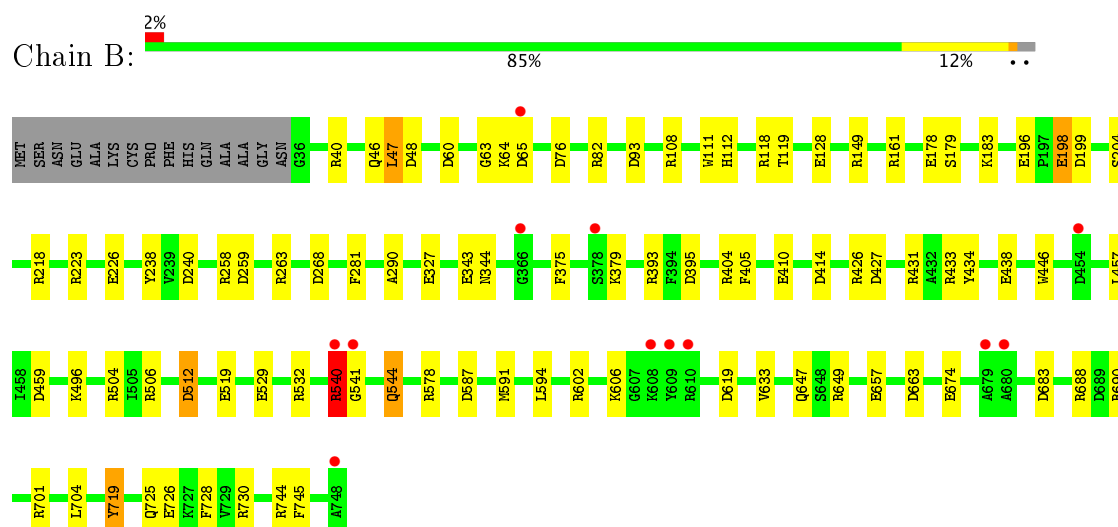
3 Residue-property plots [i](#)

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	100.84Å 115.83Å 174.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.23 – 1.70 46.23 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.6 (46.23-1.70) 95.6 (46.23-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.142 , 0.172 0.156 , 0.182	Depositor DCC
R_{free} test set	10697 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.9	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	12701	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 3.64% 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: MPD, OXY, CL, NA, PO4, ACT, 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	1.53	48/5698 (0.8%)	1.34	59/7746 (0.8%)
1	B	1.49	44/5696 (0.8%)	1.35	66/7744 (0.9%)
All	All	1.51	92/11394 (0.8%)	1.35	125/15490 (0.8%)

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196	GLU	CG-CD	9.59	1.66	1.51
1	A	198	GLU	CG-CD	9.54	1.66	1.51
1	A	544	GLN	CD-OE1	9.02	1.43	1.24
1	B	196	GLU	CG-CD	8.75	1.65	1.51
1	A	73	GLU	CG-CD	8.21	1.64	1.51
1	A	233	GLU	CD-OE2	8.15	1.34	1.25
1	B	544	GLN	CD-NE2	8.04	1.52	1.32
1	B	226	GLU	CG-CD	7.96	1.63	1.51
1	B	512	ASP	CG-OD2	7.96	1.43	1.25
1	A	434	TYR	CG-CD1	-7.92	1.28	1.39
1	A	584	GLU	CG-CD	7.88	1.63	1.51
1	A	589	GLU	CD-OE2	7.79	1.34	1.25
1	A	407	GLU	CG-CD	7.79	1.63	1.51
1	B	529	GLU	CG-CD	7.74	1.63	1.51
1	B	726	GLU	CG-CD	7.43	1.63	1.51
1	A	327	GLU	CD-OE1	7.34	1.33	1.25
1	B	161[A]	ARG	CZ-NH1	7.32	1.42	1.33
1	B	161[B]	ARG	CZ-NH1	7.32	1.42	1.33
1	A	434	TYR	CE1-CZ	-7.26	1.29	1.38
1	B	204	SER	CA-CB	7.24	1.63	1.52
1	B	410	GLU	CG-CD	7.03	1.62	1.51
1	B	540	ARG	C-O	6.95	1.36	1.23
1	B	178	GLU	CG-CD	6.89	1.62	1.51
1	B	541	GLY	C-O	6.88	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196	GLU	CB-CG	-6.75	1.39	1.52
1	A	70	GLN	CG-CD	6.72	1.66	1.51
1	A	725	GLN	CG-CD	6.71	1.66	1.51
1	A	161	ARG	CD-NE	-6.55	1.35	1.46
1	B	532	ARG	CZ-NH1	-6.55	1.24	1.33
1	B	426	ARG	CZ-NH2	6.54	1.41	1.33
1	B	446	TRP	CD2-CE2	6.46	1.49	1.41
1	A	529	GLU	CD-OE1	-6.42	1.18	1.25
1	B	196	GLU	CB-CG	-6.36	1.40	1.52
1	A	57	SER	CB-OG	6.32	1.50	1.42
1	B	82	ARG	CZ-NH2	-6.32	1.24	1.33
1	A	426[A]	ARG	CZ-NH2	6.30	1.41	1.33
1	A	426[B]	ARG	CZ-NH2	6.30	1.41	1.33
1	A	178	GLU	CG-CD	6.29	1.61	1.51
1	A	442	GLU	CD-OE2	-6.26	1.18	1.25
1	B	725	GLN	CG-CD	6.21	1.65	1.51
1	A	316	GLY	N-CA	6.21	1.55	1.46
1	B	46	GLN	CG-CD	6.20	1.65	1.51
1	A	349	GLU	CD-OE1	-6.19	1.18	1.25
1	B	719	TYR	CE1-CZ	6.12	1.46	1.38
1	B	532	ARG	CD-NE	-6.10	1.36	1.46
1	A	438	GLU	CD-OE1	-6.08	1.19	1.25
1	B	674	GLU	CG-CD	6.02	1.60	1.51
1	B	512	ASP	CB-CG	6.02	1.64	1.51
1	A	454	ASP	CB-CG	6.01	1.64	1.51
1	B	657	GLU	CD-OE2	5.99	1.32	1.25
1	B	434	TYR	CE1-CZ	-5.91	1.30	1.38
1	A	36	GLY	N-CA	5.89	1.54	1.46
1	B	438	GLU	CD-OE1	-5.89	1.19	1.25
1	B	496	LYS	CE-NZ	-5.85	1.34	1.49
1	A	589	GLU	CD-OE1	5.75	1.31	1.25
1	A	711	GLN	CD-NE2	-5.75	1.18	1.32
1	A	376	ASP	CB-CG	5.75	1.63	1.51
1	B	438	GLU	CD-OE2	5.71	1.31	1.25
1	B	63	GLY	N-CA	5.68	1.54	1.46
1	A	540	ARG	C-O	5.66	1.34	1.23
1	A	198	GLU	CD-OE2	5.56	1.31	1.25
1	A	726[A]	GLU	CD-OE1	5.54	1.31	1.25
1	A	726[B]	GLU	CD-OE1	5.54	1.31	1.25
1	A	584	GLU	CD-OE2	5.52	1.31	1.25
1	B	434	TYR	CG-CD1	-5.52	1.31	1.39
1	B	343	GLU	C-O	5.49	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	485	TRP	CE3-CZ3	5.46	1.47	1.38
1	A	245	ASP	CG-OD1	5.46	1.38	1.25
1	A	584	GLU	CD-OE1	5.46	1.31	1.25
1	A	610	ARG	CZ-NH2	5.42	1.40	1.33
1	B	223	ARG	CG-CD	-5.42	1.38	1.51
1	B	606	LYS	N-CA	5.42	1.57	1.46
1	B	410	GLU	CD-OE2	5.41	1.31	1.25
1	B	179	SER	C-O	5.38	1.33	1.23
1	B	327	GLU	CD-OE1	5.33	1.31	1.25
1	B	434	TYR	CE2-CZ	-5.33	1.31	1.38
1	A	46	GLN	CG-CD	5.33	1.63	1.51
1	A	649	ARG	CZ-NH2	-5.33	1.26	1.33
1	B	457	LEU	C-O	5.30	1.33	1.23
1	A	343	GLU	CD-OE1	5.25	1.31	1.25
1	A	688	ARG	CZ-NH2	-5.25	1.26	1.33
1	A	349	GLU	CD-OE2	-5.20	1.20	1.25
1	B	726	GLU	CD-OE2	-5.19	1.20	1.25
1	B	344	ASN	C-O	5.15	1.33	1.23
1	A	108	ARG	CZ-NH1	-5.12	1.26	1.33
1	A	407	GLU	CD-OE2	5.12	1.31	1.25
1	A	686	GLU	CG-CD	5.12	1.59	1.51
1	A	544	GLN	CG-CD	5.10	1.62	1.51
1	B	198[A]	GLU	CD-OE1	5.06	1.31	1.25
1	B	198[B]	GLU	CD-OE1	5.06	1.31	1.25
1	B	226	GLU	CB-CG	-5.06	1.42	1.52
1	A	434	TYR	CB-CG	-5.05	1.44	1.51

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	704	LEU	CB-CG-CD2	9.77	127.60	111.00
1	A	218	ARG	NE-CZ-NH2	-9.29	115.65	120.30
1	B	688	ARG	NE-CZ-NH1	9.20	124.90	120.30
1	A	40	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	A	670	ASP	CB-CG-OD2	-8.83	110.36	118.30
1	A	376	ASP	CB-CG-OD2	-8.63	110.53	118.30
1	B	108	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	B	434	TYR	CB-CG-CD1	8.55	126.13	121.00
1	B	198[A]	GLU	CG-CD-OE1	8.53	135.36	118.30
1	B	198[B]	GLU	CG-CD-OE1	8.53	135.36	118.30
1	B	431	ARG	NE-CZ-NH2	8.40	124.50	120.30
1	B	532	ARG	NE-CZ-NH1	8.39	124.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	404	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	A	263	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	A	587	ASP	CB-CG-OD1	8.19	125.67	118.30
1	B	405	PHE	CB-CG-CD2	8.18	126.53	120.80
1	B	744	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	A	48	ASP	CB-CG-OD1	8.12	125.60	118.30
1	B	82	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	A	73	GLU	OE1-CD-OE2	-8.03	113.66	123.30
1	A	258	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	B	683	ASP	CB-CG-OD2	-7.88	111.20	118.30
1	B	218	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	B	414	ASP	CB-CG-OD2	7.80	125.32	118.30
1	A	578	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	A	434	TYR	CB-CG-CD1	7.71	125.63	121.00
1	B	433	ARG	NE-CZ-NH2	-7.63	116.49	120.30
1	A	713	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	A	532	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	B	690	ARG	NE-CZ-NH2	7.27	123.93	120.30
1	A	108	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	B	258	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	A	730	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	A	258	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	A	431	ARG	NE-CZ-NH2	7.11	123.85	120.30
1	B	512	ASP	CB-CG-OD2	7.10	124.69	118.30
1	B	258	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	B	587	ASP	CB-CG-OD1	6.98	124.58	118.30
1	B	745	PHE	CB-CG-CD1	-6.93	115.95	120.80
1	B	108	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	B	719	TYR	CB-CG-CD2	-6.84	116.90	121.00
1	B	404	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	B	65	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	A	431	ARG	NE-CZ-NH1	-6.64	116.98	120.30
1	B	393	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	B	196	GLU	OE1-CD-OE2	-6.54	115.46	123.30
1	A	529	GLU	OE1-CD-OE2	-6.53	115.47	123.30
1	B	149	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	407	GLU	CG-CD-OE1	6.47	131.24	118.30
1	A	701	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	438	GLU	CG-CD-OE1	-6.44	105.41	118.30
1	A	403	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	B	540	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	B	161[A]	ARG	NE-CZ-NH2	-6.37	117.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	161[B]	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	B	504	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	A	167	ASP	CB-CG-OD2	-6.35	112.59	118.30
1	A	683	ASP	CB-CG-OD1	6.34	124.01	118.30
1	B	48	ASP	CB-CG-OD1	6.33	124.00	118.30
1	A	438	GLU	OE1-CD-OE2	6.33	130.89	123.30
1	B	259	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	B	619	ASP	CB-CG-OD1	-6.24	112.69	118.30
1	B	263	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	A	407	GLU	OE1-CD-OE2	-6.16	115.90	123.30
1	B	60	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	A	132	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	A	745	PHE	CB-CG-CD1	-6.08	116.55	120.80
1	A	744	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	B	541	GLY	N-CA-C	-5.96	98.20	113.10
1	B	395	ASP	CB-CG-OD2	5.95	123.66	118.30
1	A	47	LEU	N-CA-CB	-5.94	98.52	110.40
1	B	199	ASP	CB-CG-OD1	-5.91	112.98	118.30
1	A	454	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	433	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	B	728	PHE	CB-CG-CD1	-5.78	116.76	120.80
1	A	587	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	B	602	ARG	NE-CZ-NH1	-5.75	117.43	120.30
1	B	198[A]	GLU	CG-CD-OE2	-5.74	106.83	118.30
1	B	198[B]	GLU	CG-CD-OE2	-5.74	106.83	118.30
1	A	70	GLN	CA-CB-CG	5.73	126.01	113.40
1	A	744	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	B	47	LEU	N-CA-CB	-5.67	99.05	110.40
1	A	60	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	532	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	54	ARG	CB-CA-C	-5.60	99.20	110.40
1	A	683	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	A	240	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	B	405	PHE	CB-CG-CD1	-5.54	116.92	120.80
1	B	427	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	A	123	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	B	93	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	B	223	ARG	CA-CB-CG	-5.49	101.31	113.40
1	B	375	PHE	CB-CG-CD1	-5.48	116.96	120.80
1	B	506	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	701	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	245	ASP	CB-CG-OD2	-5.45	113.40	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	683	ASP	CB-CG-OD1	5.40	123.16	118.30
1	B	506	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	B	281	PHE	CB-CG-CD2	-5.39	117.03	120.80
1	A	610	ARG	CG-CD-NE	5.38	123.09	111.80
1	B	268	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	434	TYR	CB-CG-CD2	-5.30	117.82	121.00
1	B	240	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	376	ASP	OD1-CG-OD2	5.27	133.32	123.30
1	A	512	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	B	218	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	A	649	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	459	ASP	CB-CG-OD1	5.23	123.01	118.30
1	A	320	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	A	76	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	B	46	GLN	CA-CB-CG	5.17	124.78	113.40
1	B	76	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	B	427	ASP	CB-CG-OD1	-5.15	113.66	118.30
1	A	210	GLU	OE1-CD-OE2	-5.14	117.14	123.30
1	B	663	ASP	CB-CG-OD2	-5.14	113.68	118.30
1	A	399	GLU	CG-CD-OE2	-5.12	108.05	118.30
1	B	578	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	46	GLN	CA-CB-CG	5.11	124.64	113.40
1	A	193	ASP	CB-CG-OD1	-5.10	113.71	118.30
1	A	703	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	73	GLU	CG-CD-OE1	5.09	128.47	118.30
1	B	427	ASP	OD1-CG-OD2	5.07	132.94	123.30
1	B	459	ASP	CB-CG-OD1	5.05	122.84	118.30
1	A	416	PHE	CB-CG-CD2	5.04	124.33	120.80
1	B	223	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5550	0	5366	15	0
1	B	5542	0	5367	19	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	3	0
5	B	2	0	0	4	0
6	A	4	0	3	7	0
6	B	4	0	3	6	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
8	A	24	0	42	5	0
8	B	8	0	14	2	0
9	A	738	0	0	5	0
9	B	727	0	0	9	0
All	All	12701	0	10855	47	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 2.

All (47) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:804:OXY:O1	6:B:805:ACT:H1	1.50	1.09
1:A:119[B]:THR:HG21	9:A:1038:HOH:O	1.67	0.92
1:B:119[B]:THR:HG21	9:B:987:HOH:O	1.69	0.91
1:B:647:GLN:HG2	9:B:960:HOH:O	1.78	0.82
8:A:807:MPD:O4	8:A:807:MPD:CM	2.27	0.82
8:A:807:MPD:HM1	8:A:807:MPD:O4	1.79	0.81
1:B:112:HIS:NE2	6:B:805:ACT:C	2.43	0.81
1:A:112:HIS:NE2	6:A:805:ACT:C	2.46	0.79
1:A:520:GLN:HG2	9:A:903:HOH:O	1.85	0.77
1:B:519:GLU:OE1	9:B:901:HOH:O	2.02	0.76
5:B:804:OXY:O2	6:B:805:ACT:H1	1.86	0.74
8:A:809:MPD:HM2	8:A:809:MPD:O4	1.88	0.72
1:B:540:ARG:NE	1:B:540:ARG:HA	2.06	0.70
1:B:47:LEU:O	9:B:902:HOH:O	2.11	0.68
1:B:512:ASP:OD1	9:B:903:HOH:O	2.16	0.62
1:A:520:GLN:CG	9:A:903:HOH:O	2.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:ARG:CA	1:B:540:ARG:NE	2.63	0.59
1:B:128:GLU:OE1	1:B:198[A]:GLU:HG3	2.04	0.57
5:A:804:OXY:O1	6:A:805:ACT:CH3	2.54	0.55
1:B:591:MET:SD	1:B:594:LEU:HD12	2.45	0.55
1:A:593:VAL:HG13	9:A:929:HOH:O	2.08	0.54
1:B:540:ARG:CZ	1:B:540:ARG:HA	2.39	0.52
5:A:804:OXY:O1	6:A:805:ACT:H2	2.09	0.52
1:A:633[A]:VAL:CG2	1:A:719:TYR:CZ	2.94	0.51
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	2.95	0.50
1:B:111:TRP:HE1	6:B:805:ACT:C	2.25	0.49
5:B:804:OXY:O1	6:B:805:ACT:CH3	2.42	0.48
1:B:512:ASP:HB2	9:B:1462:HOH:O	2.14	0.48
8:A:809:MPD:O4	8:A:809:MPD:CM	2.61	0.47
1:B:730[B]:ARG:HG2	9:B:940:HOH:O	2.14	0.47
1:A:591:MET:SD	1:A:594:LEU:HD12	2.54	0.47
5:B:804:OXY:O2	9:B:904:HOH:O	2.21	0.47
1:A:111:TRP:HE1	6:A:805:ACT:C	2.27	0.46
1:A:119[A]:THR:CG2	1:A:265:ALA:HB2	2.45	0.46
1:A:112:HIS:NE2	6:A:805:ACT:O	2.49	0.46
1:A:112:HIS:CE1	6:A:805:ACT:H2	2.52	0.45
5:A:804:OXY:O2	6:A:805:ACT:H2	2.16	0.45
8:B:807:MPD:H52	8:B:807:MPD:HM1	1.98	0.45
1:B:730[A]:ARG:HD2	9:B:1498:HOH:O	2.17	0.44
1:B:290:ALA:HB2	8:B:807:MPD:H51	1.99	0.44
1:A:428:MET:O	1:A:433:ARG:HD3	2.19	0.43
1:A:426[B]:ARG:HA	1:A:426[B]:ARG:HD2	1.70	0.41
1:B:112:HIS:NE2	6:B:805:ACT:CH3	2.83	0.41
1:B:111:TRP:HZ3	1:B:238:TYR:HH	1.63	0.41
8:A:808:MPD:C1	9:A:1180:HOH:O	2.69	0.40
1:A:431:ARG:HD2	1:A:447:GLN:OE1	2.21	0.40
1:A:111:TRP:HZ3	1:A:238:TYR:HH	1.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	717/728 (98%)	706 (98%)	11 (2%)	0	100	100
1	B	717/728 (98%)	708 (99%)	9 (1%)	0	100	100
All	All	1434/1456 (98%)	1414 (99%)	20 (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	555/560 (99%)	547 (99%)	8 (1%)	71	58
1	B	555/560 (99%)	547 (99%)	8 (1%)	71	58
All	All	1110/1120 (99%)	1094 (99%)	16 (1%)	70	58

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

Mol	Chain	Res	Type
1	A	40	ARG
1	A	118	ARG
1	A	161	ARG
1	A	183	LYS
1	A	379	LYS
1	A	544	GLN
1	A	649	ARG
1	A	725	GLN
1	B	40	ARG
1	B	64	LYS
1	B	118	ARG
1	B	183	LYS
1	B	379	LYS
1	B	540	ARG
1	B	544	GLN

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Mol	Chain	Res	Type
1	B	649	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	247	ASN
1	A	520	GLN
1	B	406	HIS
1	B	647	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	2.00	7 (25%)	17,82,82	2.44	9 (52%)
5	OXY	A	804	-	1,1,1	0.36	0	0,0,0	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ACT	A	805	-	1,3,3	0.58	0	0,3,3	0.00	-
7	PO4	A	806	-	4,4,4	1.31	1 (25%)	6,6,6	2.45	2 (33%)
8	MPD	A	807	-	7,7,7	0.97	0	9,10,10	1.64	3 (33%)
8	MPD	A	808	-	7,7,7	0.88	0	9,10,10	2.29	4 (44%)
8	MPD	A	809	-	7,7,7	0.66	0	9,10,10	1.12	1 (11%)
2	HEM	B	801	1	28,50,50	1.66	5 (17%)	17,82,82	2.86	10 (58%)
5	OXY	B	804	-	1,1,1	0.30	0	0,0,0	0.00	-
6	ACT	B	805	-	1,3,3	0.00	0	0,3,3	0.00	-
7	PO4	B	806	-	4,4,4	1.27	1 (25%)	6,6,6	2.07	1 (16%)
8	MPD	B	807	-	7,7,7	0.43	0	9,10,10	1.20	1 (11%)

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	ACT	A	805	-	-	0/0/0/0	0/0/0/0
7	PO4	A	806	-	-	0/0/0/0	0/0/0/0
8	MPD	A	807	-	-	0/5/5/5	0/0/0/0
8	MPD	A	808	-	-	0/5/5/5	0/0/0/0
8	MPD	A	809	-	-	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	ACT	B	805	-	-	0/0/0/0	0/0/0/0
7	PO4	B	806	-	-	0/0/0/0	0/0/0/0
8	MPD	B	807	-	-	0/5/5/5	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C3B-C2B	-5.15	1.33	1.40
2	B	801	HEM	C1B-NB	-2.39	1.33	1.36
2	A	801	HEM	C3C-C2C	-2.39	1.37	1.40
7	B	806	PO4	P-O3	-2.07	1.47	1.54
2	A	801	HEM	C4B-NB	2.25	1.40	1.36
2	B	801	HEM	CMB-C2B	2.29	1.56	1.51
7	A	806	PO4	P-O1	2.30	1.55	1.50
2	A	801	HEM	C3B-C2B	2.41	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C1A-NA	2.51	1.41	1.36
2	A	801	HEM	CMA-C3A	2.63	1.57	1.51
2	B	801	HEM	C4A-NA	3.23	1.43	1.36
2	A	801	HEM	C3C-CAC	3.32	1.54	1.47
2	A	801	HEM	C1A-NA	3.62	1.43	1.36
2	A	801	HEM	C4D-ND	6.78	1.44	1.36

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	C1D-C2D-C3D	-6.69	102.34	107.00
7	A	806	PO4	O4-P-O1	-4.84	90.36	110.97
2	A	801	HEM	CMD-C2D-C1D	-4.65	121.31	128.46
8	A	808	MPD	CM-C2-C1	-4.64	100.06	110.42
2	B	801	HEM	CAA-CBA-CGA	-4.09	105.67	112.66
2	B	801	HEM	CMA-C3A-C4A	-4.06	122.22	128.46
2	A	801	HEM	CAA-CBA-CGA	-2.93	107.65	112.66
2	A	801	HEM	CMA-C3A-C4A	-2.48	124.65	128.46
8	A	808	MPD	O2-C2-CM	-2.32	99.95	108.00
2	B	801	HEM	CMD-C2D-C1D	-2.25	125.00	128.46
8	A	807	MPD	C1-C2-C3	-2.07	99.76	110.08
8	B	807	MPD	O4-C4-C3	-2.06	101.86	111.28
8	A	808	MPD	O2-C2-C1	2.08	115.22	108.00
2	A	801	HEM	CAD-CBD-CGD	2.09	116.23	112.66
2	B	801	HEM	CMB-C2B-C3B	2.24	129.06	124.89
2	B	801	HEM	C4A-C3A-C2A	2.25	108.56	107.00
2	B	801	HEM	CMA-C3A-C2A	2.27	129.22	124.94
8	A	809	MPD	CM-C2-C1	2.30	115.56	110.42
8	A	807	MPD	O4-C4-C5	2.33	120.17	109.46
2	A	801	HEM	CMA-C3A-C2A	2.42	129.50	124.94
2	A	801	HEM	CMC-C2C-C3C	2.47	129.48	124.89
2	B	801	HEM	CBA-CAA-C2A	2.56	117.39	112.48
2	B	801	HEM	CAD-CBD-CGD	2.63	117.16	112.66
2	A	801	HEM	CBD-CAD-C3D	2.75	117.71	112.47
2	A	801	HEM	CMB-C2B-C3B	2.92	130.30	124.89
8	A	807	MPD	CM-C2-C1	3.20	117.56	110.42
7	A	806	PO4	O3-P-O1	3.22	124.69	110.97
8	A	808	MPD	C5-C4-C3	3.24	128.24	112.11
2	B	801	HEM	CMD-C2D-C3D	4.01	132.50	124.94
2	A	801	HEM	CMD-C2D-C3D	4.05	132.57	124.94
7	B	806	PO4	O3-P-O2	4.24	123.50	107.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	804	OXY	3	0
6	A	805	ACT	7	0
8	A	807	MPD	2	0
8	A	808	MPD	1	0
8	A	809	MPD	2	0
5	B	804	OXY	4	0
6	B	805	ACT	6	0
8	B	807	MPD	2	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	713/728 (97%)	-0.41	13 (1%) 69 74	16, 23, 41, 82	0
1	B	713/728 (97%)	-0.47	12 (1%) 70 75	16, 22, 41, 82	0
All	All	1426/1456 (97%)	-0.44	25 (1%) 69 74	16, 23, 41, 82	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	540	ARG	4.8
1	A	540	ARG	4.7
1	B	610	ARG	4.1
1	B	748	ALA	3.9
1	B	541	GLY	3.8
1	A	454	ASP	3.8
1	B	679	ALA	3.8
1	A	748	ALA	3.6
1	A	541	GLY	3.6
1	B	608	LYS	3.5
1	A	215	PRO	3.2
1	B	366	GLY	2.8
1	A	542	GLY	2.5
1	B	609	TYR	2.5
1	A	680	ALA	2.3
1	A	610	ARG	2.2
1	B	65	ASP	2.2
1	A	608	LYS	2.2
1	B	378	SER	2.2
1	A	211	LEU	2.2
1	A	221	GLY	2.2
1	B	680	ALA	2.2
1	A	213	GLY	2.1
1	B	454	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	219	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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	ACT	A	805	4/4	0.89	0.42	13.67	29,31,31,33	4
8	MPD	A	807	8/8	0.90	0.15	6.10	46,60,71,74	0
8	MPD	B	807	8/8	0.84	0.18	5.48	62,68,76,81	0
2	HEM	B	801	43/43	0.99	0.11	0.61	16,17,20,24	0
2	HEM	A	801	43/43	0.98	0.09	0.39	15,18,23,25	0
3	NA	A	802	1/1	0.99	0.07	-0.93	20,20,20,20	0
4	CL	A	803	1/1	0.98	0.07	-1.41	44,44,44,44	0
3	NA	B	802	1/1	0.99	0.04	-2.01	20,20,20,20	0
4	CL	B	803	1/1	0.99	0.04	-2.42	28,28,28,28	1
7	PO4	B	806	5/5	0.94	0.18	-	41,56,58,63	0
8	MPD	A	809	8/8	0.87	0.36	-	66,74,78,81	0
8	MPD	A	808	8/8	0.91	0.17	-	35,43,53,55	0
6	ACT	B	805	4/4	0.88	0.49	-	25,27,28,34	4
5	OXY	A	804	2/2	0.92	0.09	-	36,36,36,40	0
7	PO4	A	806	5/5	0.97	0.20	-	42,53,64,66	0
5	OXY	B	804	2/2	0.96	0.08	-	32,32,32,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.