



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:37 AM UTC

PDB ID : 5V53 / pdb_00005v53
Title : Crystal structure of the D141A/Q233E/N240D variant of catalase-peroxidase from *B. pseudomallei* with acetate bound
Authors : Loewen, P.C.
Deposited on : 2017-03-13
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

<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)
Xtrriage (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

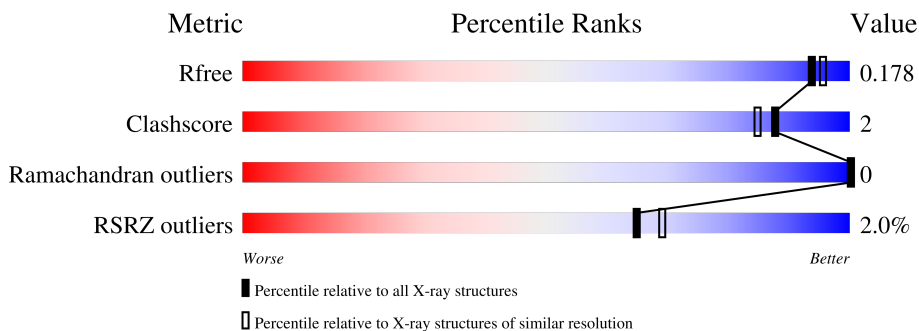
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 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	 85% 13% .
1	B	728	 84% 13% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	OXY	A	804	-	-	X	-
5	OXY	B	804	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	ACT	A	805	-	-	X	-
6	ACT	B	805	-	X	X	-
8	MPD	A	808	-	X	-	-

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		

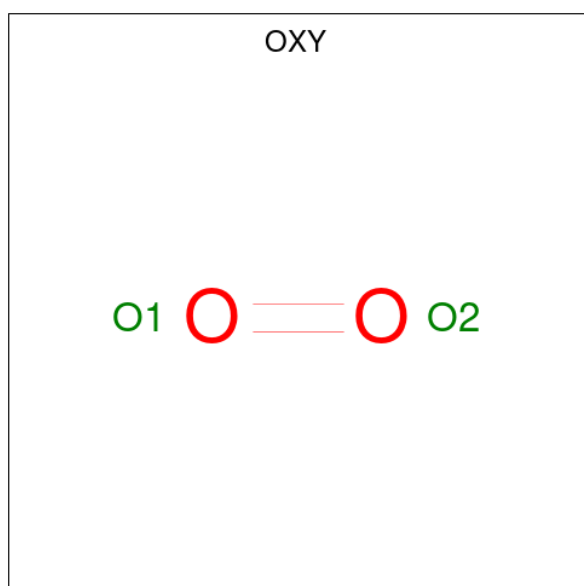
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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).



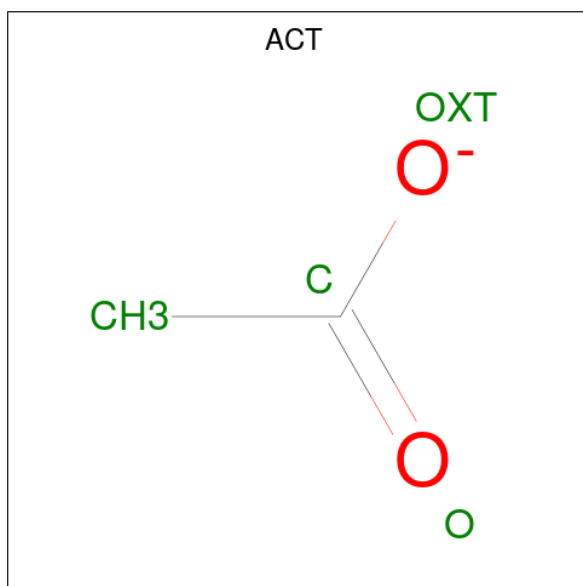
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			2	2		

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

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



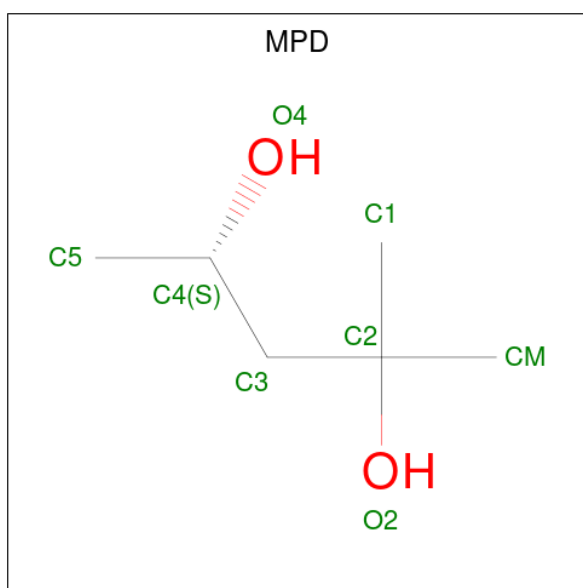
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 8 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



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

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

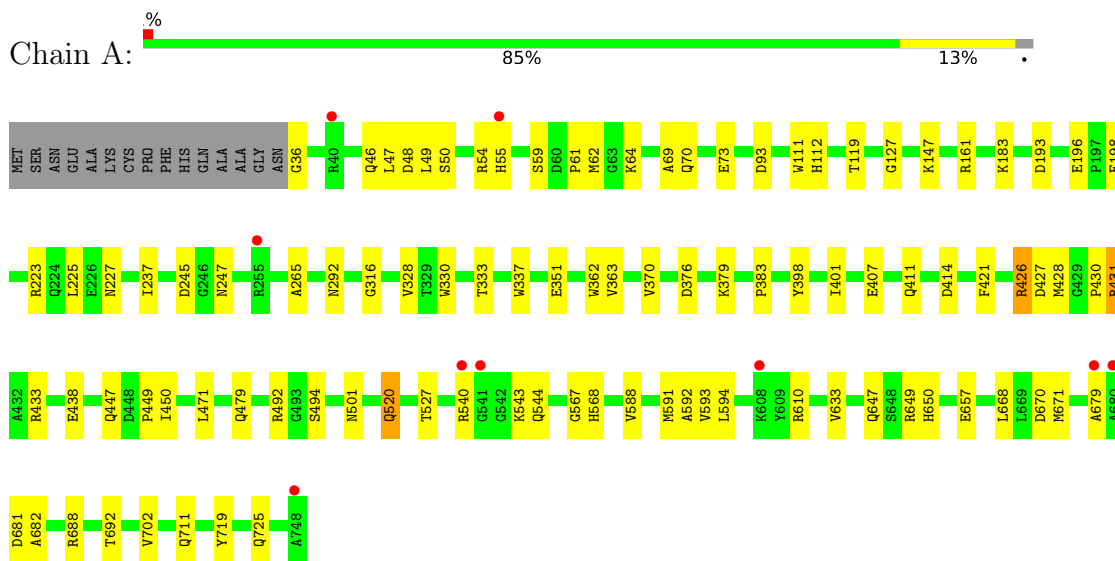
- Molecule 9 is water.

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

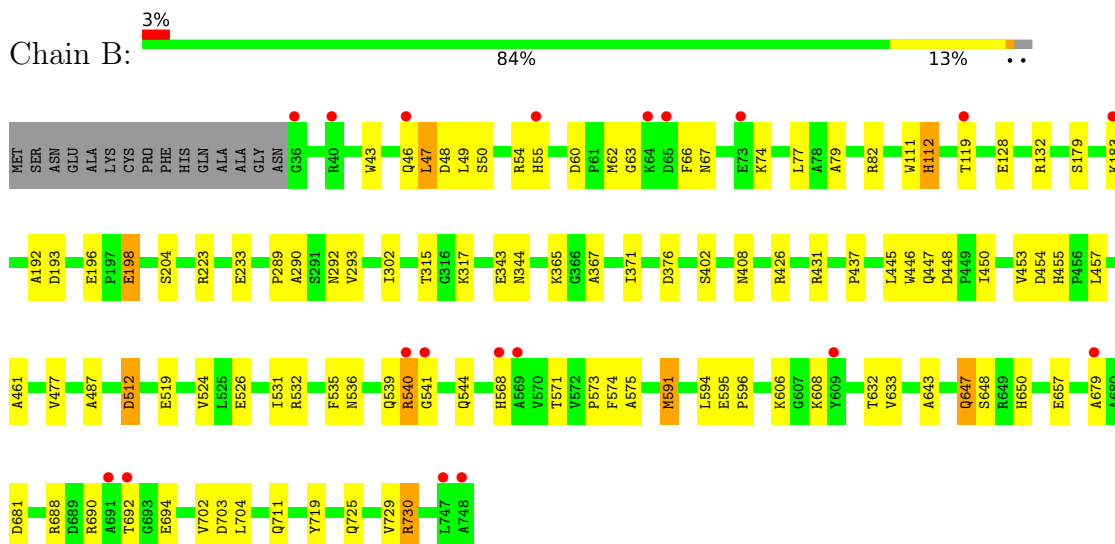
3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 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)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.142 , 0.172 (Not available) , 0.178	Depositor DCC
R_{free} test set	10704 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtrriage
Anisotropy	0.345	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NA, ACT, MPD, PO4, CL, HEM, 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	1.86	74/5698 (1.3%)	1.42	30/7746 (0.4%)
1	B	1.85	94/5696 (1.7%)	1.42	29/7744 (0.4%)
All	All	1.85	168/11394 (1.5%)	1.42	59/15490 (0.4%)

All (168) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	544	GLN	CD-OE1	10.65	1.43	1.23
1	B	540	ARG	C-O	10.38	1.36	1.23
1	B	512	ASP	CG-OD2	9.63	1.43	1.25
1	B	544	GLN	CD-NE2	9.39	1.52	1.33
1	B	606	LYS	N-CA	8.42	1.57	1.46
1	B	343	GLU	C-O	8.41	1.33	1.24
1	B	591	MET	SD-CE	-8.19	1.59	1.79
1	B	179	SER	C-O	8.03	1.33	1.24
1	A	540	ARG	C-O	8.00	1.34	1.23
1	A	161	ARG	CD-NE	-7.82	1.35	1.46
1	B	457	LEU	C-O	7.79	1.33	1.23
1	B	596	PRO	C-O	7.70	1.30	1.24
1	B	679	ALA	N-CA	7.65	1.55	1.46
1	B	344	ASN	C-O	7.59	1.33	1.24
1	B	448	ASP	C-O	7.58	1.27	1.23
1	B	54	ARG	CA-C	-7.56	1.42	1.53
1	B	448	ASP	N-CA	7.44	1.51	1.46
1	B	376	ASP	N-CA	7.41	1.55	1.46
1	B	532	ARG	CD-NE	-7.27	1.36	1.46
1	B	568	HIS	CA-C	7.25	1.61	1.52
1	B	371	ILE	N-CA	7.24	1.55	1.46
1	B	63	GLY	N-CA	7.19	1.54	1.45
1	A	647	GLN	CA-C	7.11	1.62	1.53
1	A	427	ASP	CA-C	-7.05	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	711	GLN	CD-NE2	-7.04	1.18	1.33
1	A	328	VAL	C-O	7.02	1.31	1.24
1	B	455	HIS	CA-C	7.02	1.60	1.52
1	A	588	VAL	N-CA	-6.97	1.37	1.46
1	B	60	ASP	CA-C	-6.96	1.44	1.52
1	A	688	ARG	CA-C	-6.93	1.44	1.52
1	A	679	ALA	N-CA	6.92	1.54	1.46
1	B	198[A]	GLU	C-O	6.92	1.32	1.23
1	B	198[B]	GLU	C-O	6.92	1.32	1.23
1	A	471	LEU	CA-C	6.91	1.62	1.52
1	B	47	LEU	CB-CG	-6.89	1.39	1.53
1	B	192	ALA	N-CA	6.88	1.54	1.46
1	A	383	PRO	CA-C	-6.83	1.44	1.52
1	B	408	ASN	CA-CB	-6.69	1.45	1.53
1	A	316	GLY	N-CA	6.66	1.55	1.45
1	B	82	ARG	CZ-NH2	-6.63	1.24	1.33
1	A	376	ASP	N-CA	6.62	1.54	1.46
1	A	245	ASP	CG-OD1	6.61	1.38	1.25
1	B	535	PHE	CA-C	-6.61	1.44	1.52
1	A	362	TRP	CA-C	-6.57	1.44	1.52
1	A	692	THR	CA-C	-6.56	1.44	1.52
1	A	193	ASP	C-O	6.52	1.32	1.23
1	B	681	ASP	CA-C	6.51	1.59	1.52
1	B	692	THR	N-CA	6.48	1.54	1.46
1	A	363	VAL	C-O	6.41	1.30	1.24
1	B	573	PRO	CA-C	6.40	1.60	1.52
1	B	596	PRO	C-N	-6.39	1.26	1.33
1	B	315	THR	CA-C	6.37	1.61	1.52
1	A	398	TYR	C-O	6.34	1.31	1.24
1	B	55	HIS	CA-CB	6.34	1.63	1.53
1	B	204	SER	CA-CB	6.28	1.63	1.53
1	B	426	ARG	CZ-NH2	6.23	1.41	1.33
1	A	527	THR	N-CA	-6.20	1.39	1.46
1	B	541	GLY	C-O	6.20	1.34	1.23
1	A	431	ARG	N-CA	6.16	1.54	1.46
1	B	461	ALA	CA-C	6.14	1.60	1.52
1	B	55	HIS	C-O	-6.05	1.15	1.23
1	A	568	HIS	CA-C	6.03	1.59	1.52
1	B	365	LYS	N-CA	6.00	1.53	1.46
1	A	237	ILE	C-O	5.99	1.29	1.24
1	A	682	ALA	CA-C	5.99	1.60	1.52
1	B	79	ALA	N-CA	-5.99	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	647	GLN	CA-C	5.99	1.61	1.53
1	A	670	ASP	CA-CB	5.97	1.60	1.53
1	A	46	GLN	N-CA	5.95	1.53	1.45
1	A	47	LEU	CB-CG	-5.92	1.41	1.53
1	B	532	ARG	CZ-NH1	-5.87	1.24	1.32
1	A	61	PRO	N-CA	-5.84	1.39	1.47
1	A	449	PRO	CA-C	5.84	1.60	1.52
1	B	292	ASN	CA-C	5.84	1.60	1.52
1	A	36	GLY	N-CA	5.84	1.54	1.45
1	B	437	PRO	CA-C	-5.79	1.46	1.52
1	A	70	GLN	CG-CD	5.78	1.66	1.52
1	A	69	ALA	CA-C	-5.77	1.44	1.52
1	A	725	GLN	CG-CD	5.77	1.66	1.52
1	B	402	SER	N-CA	-5.74	1.39	1.46
1	A	351	GLU	C-O	5.73	1.31	1.24
1	B	703	ASP	N-CA	-5.73	1.39	1.46
1	B	431	ARG	N-CA	5.73	1.53	1.46
1	A	225	LEU	CA-CB	5.73	1.61	1.53
1	A	196	GLU	CG-CD	5.71	1.66	1.52
1	A	49	LEU	N-CA	-5.70	1.38	1.46
1	A	198	GLU	CG-CD	5.68	1.66	1.52
1	B	447	GLN	CA-C	5.68	1.62	1.52
1	B	74	LYS	CA-C	5.68	1.60	1.52
1	B	67	ASN	CA-C	5.66	1.59	1.52
1	B	112	HIS	C-O	5.64	1.31	1.24
1	A	649	ARG	CZ-NH2	-5.64	1.26	1.33
1	A	292	ASN	CA-C	5.62	1.60	1.52
1	B	77	LEU	CA-CB	-5.61	1.44	1.53
1	B	650	HIS	CA-C	5.61	1.60	1.52
1	A	47	LEU	CA-C	5.59	1.60	1.52
1	B	367	ALA	N-CA	-5.59	1.38	1.45
1	A	227	ASN	CA-C	-5.58	1.47	1.53
1	B	730[A]	ARG	N-CA	-5.57	1.39	1.46
1	B	730[B]	ARG	N-CA	-5.57	1.39	1.46
1	A	688	ARG	CZ-NH2	-5.56	1.26	1.33
1	B	688	ARG	N-CA	5.54	1.52	1.45
1	B	453	VAL	C-O	-5.54	1.17	1.24
1	B	729	VAL	N-CA	5.53	1.53	1.46
1	B	575	ALA	C-O	-5.53	1.20	1.25
1	A	64	LYS	C-O	-5.52	1.16	1.24
1	B	526	GLU	N-CA	5.51	1.53	1.46
1	A	671	MET	CA-C	5.49	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	711	GLN	CD-NE2	-5.48	1.21	1.33
1	A	370	VAL	CA-C	5.44	1.58	1.52
1	B	487	ALA	N-CA	-5.44	1.39	1.46
1	A	520	GLN	CA-C	5.43	1.59	1.52
1	B	46	GLN	N-CA	5.43	1.53	1.45
1	A	567	GLY	C-O	-5.40	1.17	1.24
1	A	421	PHE	N-CA	5.40	1.52	1.46
1	A	650	HIS	N-CA	5.39	1.53	1.46
1	A	59	SER	C-O	-5.39	1.17	1.24
1	A	93	ASP	CA-C	-5.34	1.45	1.52
1	A	692	THR	N-CA	5.34	1.53	1.46
1	B	725	GLN	CG-CD	5.31	1.65	1.52
1	B	46	GLN	CG-CD	5.30	1.65	1.52
1	B	376	ASP	CA-C	-5.29	1.46	1.52
1	A	426[A]	ARG	CZ-NH2	5.29	1.40	1.33
1	A	426[B]	ARG	CZ-NH2	5.29	1.40	1.33
1	B	49	LEU	CB-CG	-5.29	1.42	1.53
1	A	147	LYS	C-O	-5.28	1.17	1.24
1	B	293	VAL	N-CA	5.26	1.52	1.46
1	B	632	THR	CA-CB	5.25	1.61	1.53
1	B	289	PRO	N-CA	-5.23	1.40	1.47
1	B	193	ASP	C-O	5.23	1.30	1.23
1	B	643	ALA	CA-C	5.22	1.59	1.52
1	B	650	HIS	CA-CB	-5.21	1.45	1.53
1	B	544	GLN	CA-C	5.21	1.59	1.52
1	B	196	GLU	CG-CD	5.21	1.65	1.52
1	B	702	VAL	N-CA	5.19	1.52	1.46
1	B	608	LYS	N-CA	5.18	1.52	1.46
1	A	55	HIS	CA-CB	5.18	1.61	1.53
1	B	524	VAL	CA-C	-5.18	1.46	1.52
1	A	379	LYS	CA-C	5.18	1.58	1.52
1	B	302	ILE	CB-CG1	-5.17	1.43	1.53
1	B	574	PHE	CA-CB	-5.17	1.45	1.53
1	B	694	GLU	CA-C	5.17	1.59	1.52
1	A	127	GLY	C-O	5.16	1.29	1.24
1	B	657	GLU	CA-C	5.16	1.59	1.52
1	B	43	TRP	CA-CB	5.14	1.60	1.53
1	B	531	ILE	N-CA	5.14	1.52	1.46
1	A	657	GLU	CA-C	5.14	1.59	1.52
1	B	454	ASP	CA-CB	5.13	1.60	1.53
1	A	543	LYS	N-CA	5.13	1.52	1.46
1	A	247	ASN	CG-ND2	-5.13	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	430	PRO	N-CA	5.12	1.53	1.47
1	A	610	ARG	CZ-NH2	5.12	1.40	1.33
1	B	477	VAL	N-CA	5.11	1.52	1.46
1	B	317	LYS	CA-CB	-5.10	1.45	1.53
1	A	337	TRP	CA-C	5.09	1.59	1.52
1	B	317	LYS	N-CA	5.07	1.51	1.46
1	A	681	ASP	CA-C	5.07	1.58	1.52
1	B	532	ARG	N-CA	-5.06	1.40	1.46
1	B	233	GLU	CA-C	5.06	1.58	1.52
1	A	702	VAL	CA-CB	5.04	1.61	1.54
1	A	492	ARG	C-O	5.04	1.29	1.23
1	B	132	ARG	CA-C	5.04	1.59	1.52
1	A	401	ILE	CA-C	5.03	1.59	1.52
1	B	536	ASN	CA-C	5.01	1.59	1.52
1	A	414	ASP	CG-OD1	-5.01	1.15	1.25
1	A	501	ASN	CA-C	5.01	1.59	1.52
1	A	333	THR	CA-C	5.01	1.58	1.52
1	A	494	SER	CA-CB	-5.01	1.45	1.53

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	GLU	CB-CG-CD	8.74	127.46	112.60
1	A	47	LEU	N-CA-CB	-7.79	98.52	109.97
1	B	47	LEU	N-CA-CB	-7.72	99.05	110.17
1	B	48	ASP	N-CA-C	7.39	121.50	107.75
1	B	725	GLN	CB-CG-CD	7.05	124.59	112.60
1	B	445	LEU	N-CA-C	6.84	119.58	111.71
1	B	46	GLN	N-CA-C	-6.84	101.47	110.43
1	B	62	MET	CA-C-N	-6.74	112.91	120.53
1	B	62	MET	C-N-CA	-6.74	112.91	120.53
1	A	46	GLN	N-CA-C	-6.66	101.71	110.43
1	B	541	GLY	N-CA-C	-6.47	98.20	112.17
1	B	223	ARG	CA-CB-CG	-6.39	101.31	114.10
1	A	48	ASP	N-CA-C	6.19	119.82	107.62
1	B	66	PHE	CA-C-N	-6.19	114.07	122.86
1	B	66	PHE	C-N-CA	-6.19	114.07	122.86
1	B	446	TRP	CA-C-O	6.18	126.98	119.38
1	A	330	TRP	N-CA-C	6.14	119.24	111.69
1	A	479	GLN	N-CA-C	6.09	117.59	111.07
1	B	595	GLU	O-C-N	6.04	126.67	121.30
1	A	544	GLN	CG-CD-NE2	-6.04	107.35	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	ARG	CB-CA-C	-5.99	99.20	110.51
1	A	70	GLN	CA-CB-CG	5.96	126.01	114.10
1	B	431	ARG	NE-CZ-NH2	5.89	124.50	119.20
1	A	592	ALA	N-CA-C	5.87	118.43	111.33
1	B	539	GLN	O-C-N	5.80	129.46	122.85
1	B	540	ARG	CA-C-O	5.74	127.65	121.16
1	A	62	MET	CA-C-N	-5.70	112.91	121.01
1	A	62	MET	C-N-CA	-5.70	112.91	121.01
1	B	50	SER	CA-CB-OG	-5.67	99.76	111.10
1	B	571[A]	THR	CA-C-O	5.66	126.55	120.38
1	B	571[B]	THR	CA-C-O	5.66	126.55	120.38
1	A	438	GLU	CG-CD-OE1	-5.65	105.41	118.40
1	B	704	LEU	CB-CG-CD2	5.63	127.60	110.70
1	B	450	ILE	CB-CA-C	-5.59	104.32	110.52
1	A	407	GLU	CG-CD-OE1	5.58	131.24	118.40
1	A	183	LYS	CB-CG-CD	5.57	124.12	111.30
1	A	450	ILE	CB-CA-C	-5.57	104.34	110.52
1	A	407	GLU	CB-CG-CD	5.55	122.03	112.60
1	B	54	ARG	CA-C-N	-5.47	114.87	122.74
1	B	54	ARG	C-N-CA	-5.47	114.87	122.74
1	A	223	ARG	CA-CB-CG	-5.46	103.19	114.10
1	A	55	HIS	CB-CA-C	5.45	119.84	111.39
1	A	198	GLU	N-CA-CB	5.38	118.47	110.29
1	B	647	GLN	N-CA-CB	-5.34	104.01	112.08
1	B	46	GLN	CA-CB-CG	5.34	124.78	114.10
1	A	73	GLU	CB-CG-CD	5.31	121.62	112.60
1	B	183	LYS	CG-CD-CE	5.30	123.49	111.30
1	A	50	SER	CA-CB-OG	-5.29	100.53	111.10
1	A	46	GLN	CA-CB-CG	5.27	124.64	114.10
1	B	690	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	A	668	LEU	CD1-CG-CD2	5.24	122.32	110.80
1	B	446	TRP	O-C-N	-5.23	115.42	122.43
1	A	411	GLN	N-CA-C	-5.22	105.67	111.36
1	A	431	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	A	46	GLN	CB-CG-CD	5.09	121.25	112.60
1	B	648	SER	N-CA-C	-5.05	103.12	110.24
1	A	610	ARG	CG-CD-NE	5.04	123.09	112.00
1	A	438	GLU	CA-C-O	5.02	126.02	119.95
1	A	46	GLN	N-CA-CB	5.00	117.42	110.26

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	14	0
1	B	5542	0	5367	18	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	45	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 (45) 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:O4	8:A:807:MPD:HM1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O4	8:A:809:MPD:HM2	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
1:B:540:ARG:NE	1:B:540:ARG:CA	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:HA	1:B:540:ARG:CZ	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:HM1	8:B:807:MPD:H52	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
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

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 [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 oligosaccharides 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
8	MPD	A	809	-	7,7,7	0.73	0	9,10,10	1.18	2 (22%)
6	ACT	B	805	-	3,3,3	1.67	1 (33%)	3,3,3	2.35	2 (66%)
5	OXY	B	804	-	1,1,1	0.41	0	-		
2	HEM	A	801	1	50,50,50	1.73	12 (24%)	67,82,82	1.45	16 (23%)
8	MPD	A	807	-	7,7,7	1.04	0	9,10,10	1.73	3 (33%)
6	ACT	A	805	-	3,3,3	1.64	1 (33%)	3,3,3	0.78	0
8	MPD	A	808	-	7,7,7	0.98	0	9,10,10	2.45	4 (44%)
7	PO4	B	806	-	4,4,4	1.48	1 (25%)	6,6,6	2.45	2 (33%)
7	PO4	A	806	-	4,4,4	1.30	1 (25%)	6,6,6	2.94	2 (33%)
2	HEM	B	801	1	50,50,50	1.50	8 (16%)	67,82,82	1.53	13 (19%)
5	OXY	A	804	-	1,1,1	0.46	0	-		
8	MPD	B	807	-	7,7,7	0.48	0	9,10,10	1.30	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
8	MPD	A	809	-	-	3/5/5/5	-
2	HEM	A	801	1	-	3/14/54/54	-
8	MPD	A	807	-	-	0/5/5/5	-
8	MPD	A	808	-	-	5/5/5/5	-
2	HEM	B	801	1	-	3/14/54/54	-
8	MPD	B	807	-	-	3/5/5/5	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C4A-NA	-4.12	1.31	1.39
2	A	801	HEM	FE-NC	3.75	2.07	1.95
2	B	801	HEM	C1B-NB	-3.64	1.33	1.40
2	A	801	HEM	FE-NB	3.51	2.05	1.94
2	B	801	HEM	FE-NB	3.51	2.05	1.94
2	A	801	HEM	FE-NA	3.31	2.06	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C3B-C2B	3.14	1.43	1.37
2	A	801	HEM	CMA-C3A	3.03	1.57	1.50
2	B	801	HEM	CHB-C1B	2.80	1.44	1.38
6	B	805	ACT	O-C	2.79	1.34	1.22
2	B	801	HEM	CMB-C2B	2.78	1.56	1.50
6	A	805	ACT	O-C	2.69	1.34	1.22
2	A	801	HEM	C4D-ND	2.65	1.44	1.40
7	B	806	PO4	P-O3	-2.60	1.47	1.54
2	A	801	HEM	CAC-C3C	2.60	1.54	1.47
2	A	801	HEM	C3B-C4B	2.38	1.49	1.44
2	B	801	HEM	O2A-CGA	-2.29	1.23	1.30
2	B	801	HEM	FE-NC	2.29	2.02	1.95
2	A	801	HEM	C1A-NA	2.28	1.43	1.39
2	A	801	HEM	C1A-C2A	-2.23	1.40	1.44
2	A	801	HEM	C1C-NC	-2.06	1.35	1.39
7	A	806	PO4	P-O1	2.04	1.55	1.50
2	B	801	HEM	C1C-NC	-2.02	1.35	1.39
2	B	801	HEM	O1D-CGD	2.01	1.28	1.22

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	806	PO4	O4-P-O1	-5.82	90.36	110.95
7	B	806	PO4	O3-P-O2	5.01	123.50	107.91
8	A	808	MPD	CM-C2-C1	-4.72	100.06	110.63
2	B	801	HEM	C1D-C2D-C3D	-4.41	102.34	106.98
7	A	806	PO4	O3-P-O1	3.88	124.69	110.95
2	B	801	HEM	CHC-C1C-NC	3.60	128.37	124.45
8	A	808	MPD	C5-C4-C3	3.57	128.24	111.67
2	A	801	HEM	C1B-NB-C4B	3.40	109.23	105.21
2	B	801	HEM	CHB-C4A-NA	-3.38	117.73	123.86
2	A	801	HEM	C3D-C4D-ND	-3.20	106.67	110.17
6	B	805	ACT	OXT-C-CH3	3.13	128.19	115.05
2	A	801	HEM	O1A-CGA-CBA	-3.10	113.26	123.09
8	A	807	MPD	CM-C2-C1	3.10	117.56	110.63
2	B	801	HEM	CHC-C1C-C2C	-3.03	119.19	125.49
2	B	801	HEM	CAA-CBA-CGA	-3.02	105.67	113.67
2	B	801	HEM	CMC-C2C-C1C	2.59	129.29	124.73
8	A	808	MPD	O2-C2-CM	-2.58	99.95	107.99
2	B	801	HEM	C3B-C4B-NB	-2.50	107.67	109.47
8	A	807	MPD	O4-C4-C5	2.49	120.17	109.45
2	A	801	HEM	C4D-C3D-C2D	2.46	110.48	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	C4B-C3B-C2B	-2.44	105.04	107.28
2	A	801	HEM	C3B-C4B-NB	-2.43	107.72	109.47
8	A	807	MPD	C1-C2-C3	-2.42	99.76	110.20
2	A	801	HEM	O2A-CGA-CBA	2.41	121.61	114.00
7	B	806	PO4	O4-P-O1	-2.40	102.47	110.95
8	B	807	MPD	O4-C4-C3	-2.39	101.86	111.35
2	A	801	HEM	CMD-C2D-C1D	-2.38	121.31	125.03
2	A	801	HEM	CMD-C2D-C3D	2.37	132.57	126.15
2	A	801	HEM	CAD-C3D-C2D	-2.35	123.46	127.87
2	B	801	HEM	CMD-C2D-C3D	2.35	132.50	126.15
2	B	801	HEM	C4A-NA-C1A	-2.33	102.02	105.82
8	A	808	MPD	O2-C2-C1	2.32	115.22	107.99
2	A	801	HEM	CAA-CBA-CGA	-2.27	107.65	113.67
2	B	801	HEM	C1B-NB-C4B	2.26	107.88	105.21
8	A	809	MPD	CM-C2-C1	2.20	115.56	110.63
2	A	801	HEM	C3C-C2C-C1C	-2.18	104.99	107.05
2	A	801	HEM	CMB-C2B-C1B	-2.16	121.66	125.03
2	A	801	HEM	C3B-C2B-C1B	2.14	108.02	106.41
8	A	809	MPD	O2-C2-CM	-2.13	101.34	107.99
2	A	801	HEM	CHC-C4B-NB	2.10	126.69	124.42
2	B	801	HEM	CMA-C3A-C4A	-2.10	122.22	125.42
6	B	805	ACT	OXT-C-O	-2.09	114.28	122.03
2	A	801	HEM	O2D-CGD-CBD	2.06	120.50	114.00
2	B	801	HEM	CAD-C3D-C2D	-2.05	124.03	127.87
2	B	801	HEM	O1A-CGA-CBA	-2.04	116.62	123.09

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	808	MPD	C1-C2-C3-C4
8	A	808	MPD	C2-C3-C4-C5
8	A	809	MPD	C2-C3-C4-C5
8	B	807	MPD	C2-C3-C4-O4
8	B	807	MPD	C2-C3-C4-C5
8	A	808	MPD	O2-C2-C3-C4
8	A	808	MPD	CM-C2-C3-C4
2	B	801	HEM	CAA-CBA-CGA-O2A
2	A	801	HEM	CAA-CBA-CGA-O2A
2	A	801	HEM	CAA-CBA-CGA-O1A
2	B	801	HEM	CAA-CBA-CGA-O1A
8	A	809	MPD	O2-C2-C3-C4

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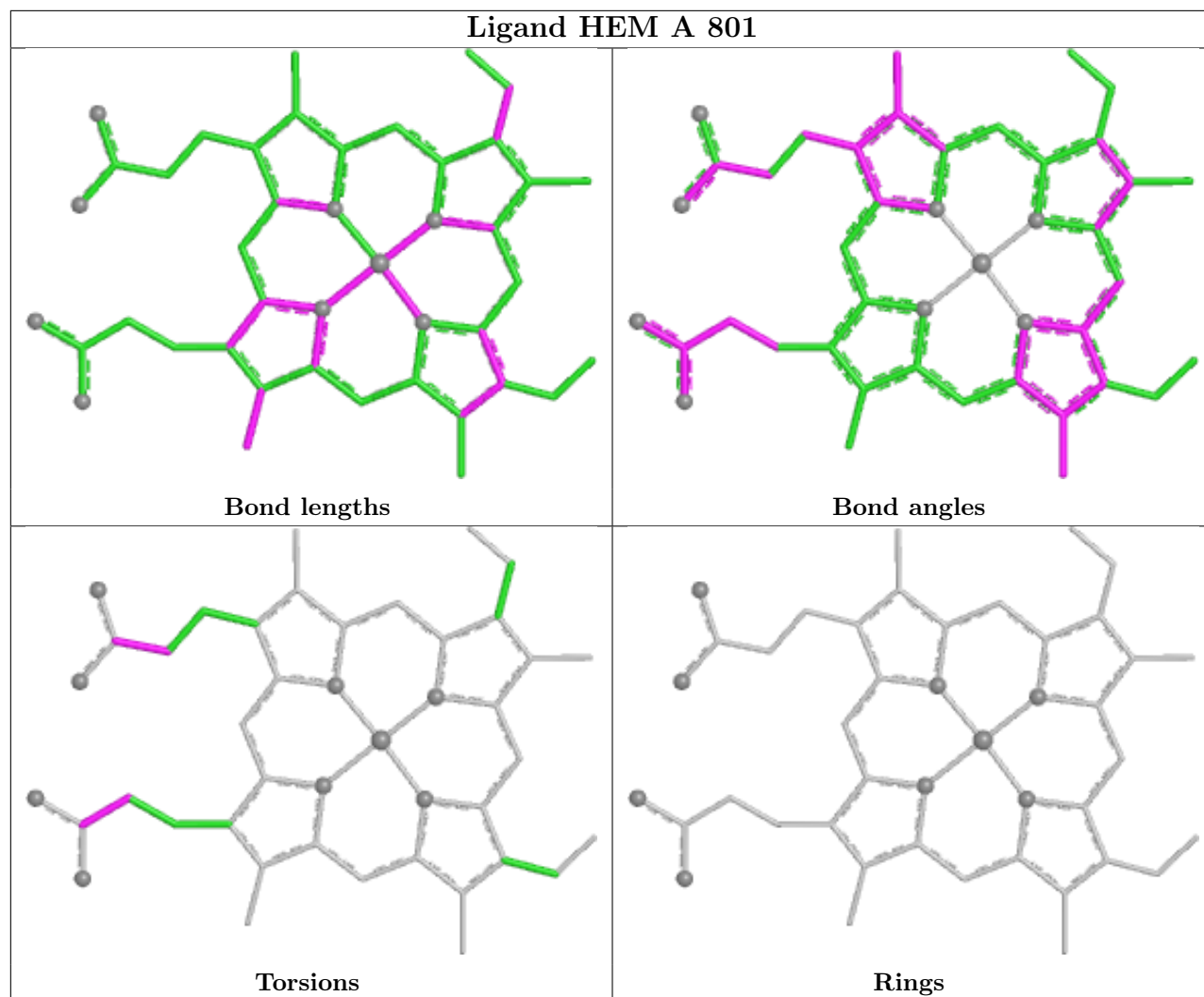
Mol	Chain	Res	Type	Atoms
8	A	808	MPD	C2-C3-C4-O4
8	A	809	MPD	C2-C3-C4-O4
8	B	807	MPD	C1-C2-C3-C4
2	B	801	HEM	CAD-CBD-CGD-O2D
2	A	801	HEM	CAD-CBD-CGD-O2D

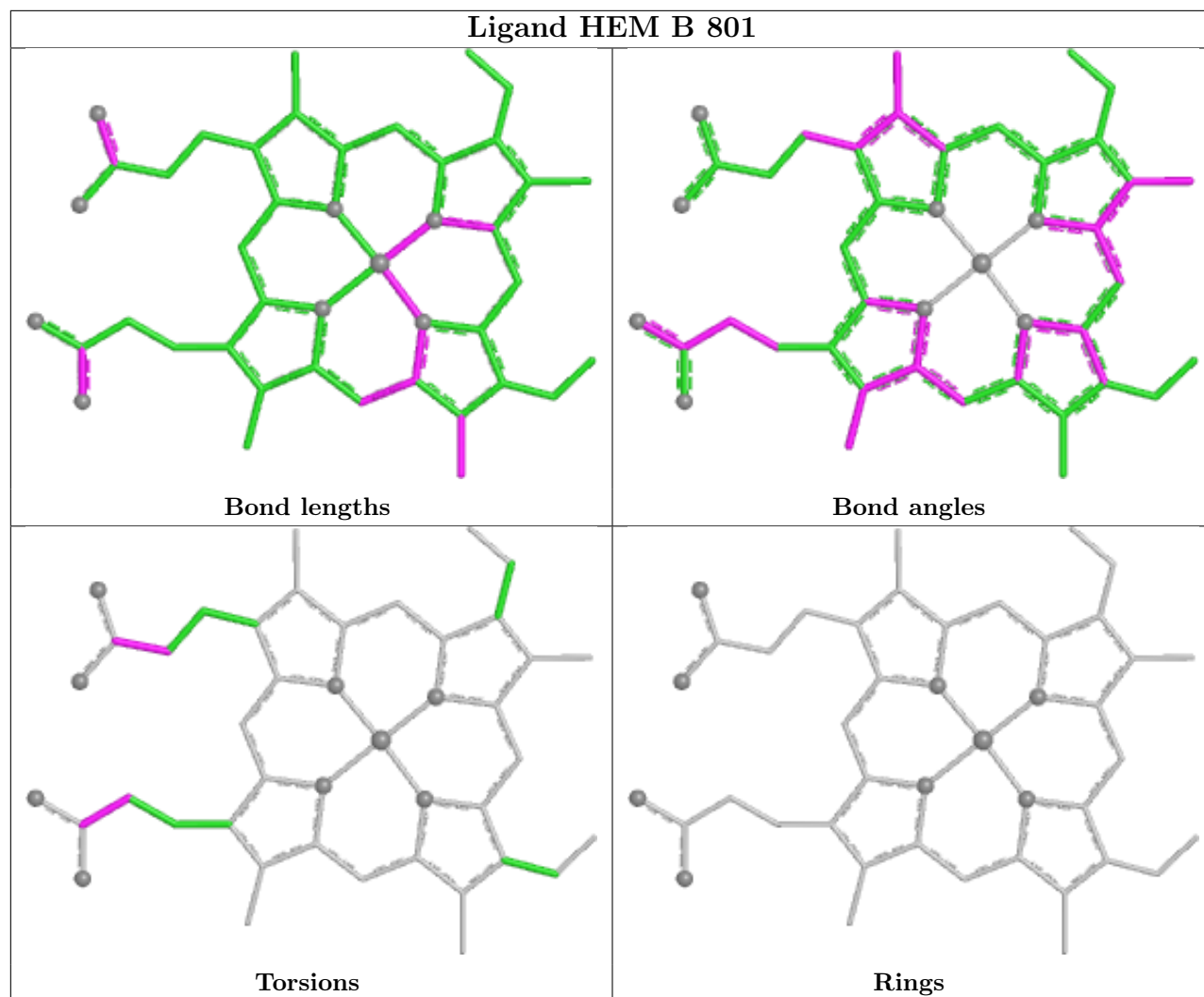
There are no ring outliers.

8 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	809	MPD	2	0
6	B	805	ACT	6	0
5	B	804	OXY	4	0
8	A	807	MPD	2	0
6	A	805	ACT	7	0
8	A	808	MPD	1	0
5	A	804	OXY	3	0
8	B	807	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	713/728 (97%)	-0.23	9 (1%) 75 79	9, 23, 41, 82	6 (0%)
1	B	713/728 (97%)	-0.29	19 (2%) 56 60	9, 22, 41, 82	6 (0%)
All	All	1426/1456 (97%)	-0.26	28 (1%) 65 69	9, 23, 41, 82	12 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	748	ALA	4.3
1	A	748	ALA	4.0
1	B	55	HIS	3.5
1	B	40	ARG	2.9
1	A	40	ARG	2.8
1	B	36	GLY	2.8
1	B	541	GLY	2.7
1	B	73	GLU	2.6
1	B	65	ASP	2.6
1	A	540	ARG	2.6
1	A	541	GLY	2.5
1	A	680	ALA	2.5
1	A	608	LYS	2.4
1	B	691	ALA	2.3
1	B	692	THR	2.3
1	B	540	ARG	2.3
1	B	46	GLN	2.3
1	A	55	HIS	2.3
1	A	679	ALA	2.2
1	B	679	ALA	2.2
1	B	747	LEU	2.2
1	B	183	LYS	2.2
1	B	64	LYS	2.2
1	B	609	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	569	ALA	2.1
1	B	119[A]	THR	2.1
1	A	255[A]	ARG	2.1
1	B	568	HIS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

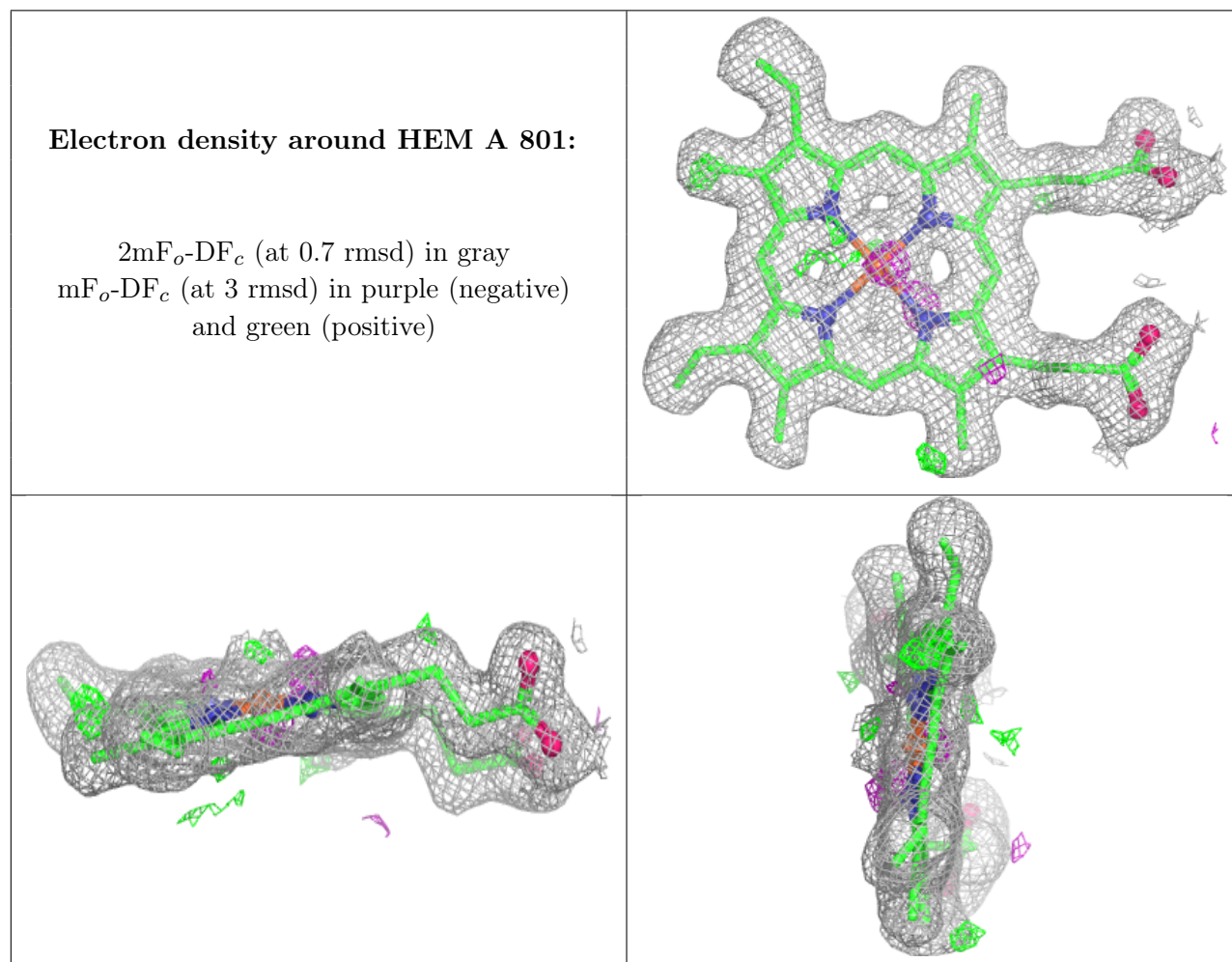
6.4 Ligands [i](#)

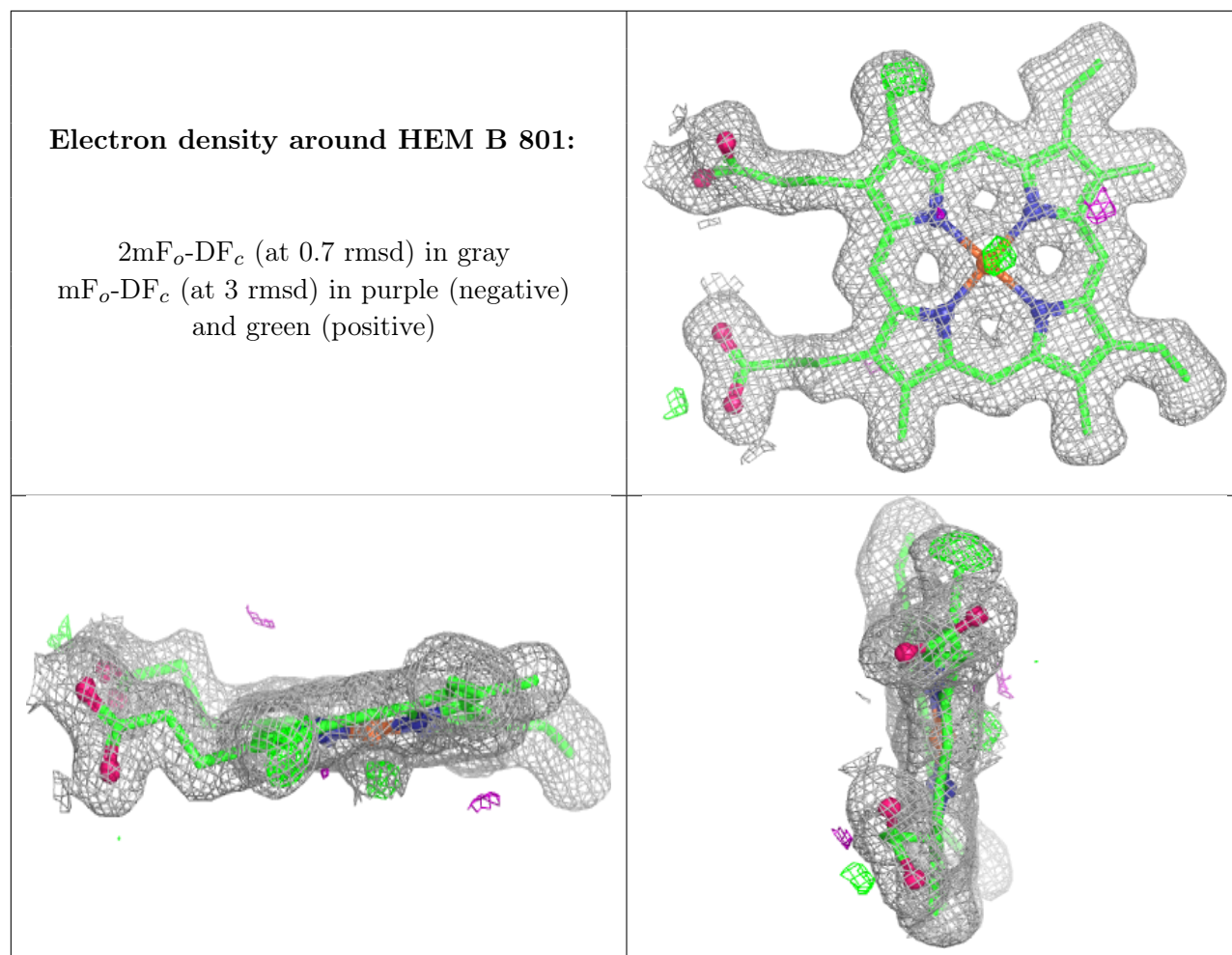
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	MPD	A	809	8/8	0.83	0.21	66,74,78,81	0
8	MPD	B	807	8/8	0.85	0.17	62,68,76,81	0
8	MPD	A	808	8/8	0.88	0.14	35,43,53,55	0
6	ACT	A	805	4/4	0.88	0.23	29,31,31,33	4
8	MPD	A	807	8/8	0.88	0.17	46,60,71,74	0
6	ACT	B	805	4/4	0.89	0.21	25,27,28,34	4
7	PO4	B	806	5/5	0.91	0.10	41,56,58,63	0
5	OXY	A	804	2/2	0.92	0.19	36,36,36,40	0
4	CL	A	803	1/1	0.92	0.12	44,44,44,44	0
7	PO4	A	806	5/5	0.93	0.07	42,53,64,66	0
5	OXY	B	804	2/2	0.94	0.14	32,32,32,34	0
4	CL	B	803	1/1	0.98	0.09	28,28,28,28	1
2	HEM	A	801	43/43	0.99	0.04	15,18,23,25	0
2	HEM	B	801	43/43	0.99	0.04	16,17,20,24	0
3	NA	A	802	1/1	0.99	0.03	20,20,20,20	0
3	NA	B	802	1/1	0.99	0.06	20,20,20,20	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.





6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.