



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:14 AM GMT

PDB ID : 2CAH
Title : STRUCTURE OF PROTEUS MIRABILIS PR CATALASE FOR THE NATIVE FORM (E-FE(III)) COMPLEXED WITH NADPH
Authors : Gouet, P.; Jouve, H.-M.; Dideberg, O.
Deposited on : 1996-07-01
Resolution : 2.70 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

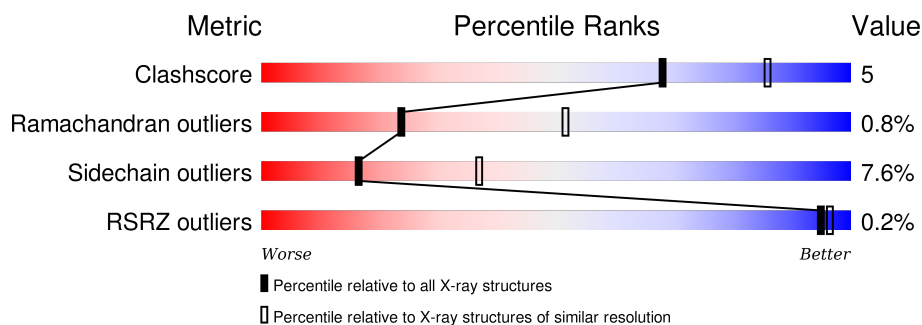
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.70 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))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	484	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4045 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	28	0	0
			3861	2447	684	715	15			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	OMT	MET	MODIFIED RESIDUE	UNP P42321

- 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		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	48	21	7	17	3	0	0

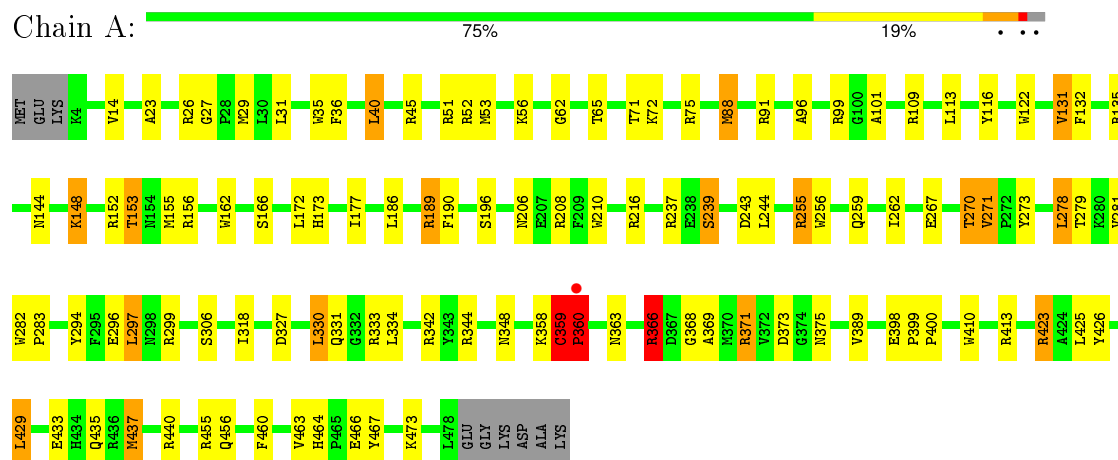
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	93	Total	0	0
			93 O		

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 errors 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



4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	112.36Å 112.36Å 249.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.70 14.86 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.0 (15.00-2.70) 91.0 (14.86-2.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.97 (at 2.69Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.196 , (Not available) 0.177 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 54.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 23830 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4045	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NDP, OMT, 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	0.91	0/3961	1.70	79/5359 (1.5%)

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

There are no bond length outliers.

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	371	ARG	NE-CZ-NH1	19.89	130.24	120.30
1	A	371	ARG	NE-CZ-NH2	-15.54	112.53	120.30
1	A	189	ARG	NE-CZ-NH1	12.51	126.56	120.30
1	A	135	ARG	NE-CZ-NH1	12.14	126.37	120.30
1	A	440	ARG	NE-CZ-NH2	-11.94	114.33	120.30
1	A	440	ARG	NE-CZ-NH1	11.73	126.17	120.30
1	A	135	ARG	NE-CZ-NH2	-10.23	115.18	120.30
1	A	131	VAL	CG1-CB-CG2	-9.68	95.41	110.90
1	A	423	ARG	NE-CZ-NH1	9.27	124.94	120.30
1	A	210	TRP	CE2-CD2-CG	-9.24	99.91	107.30
1	A	256	TRP	CD1-CG-CD2	9.22	113.68	106.30
1	A	333	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	A	162	TRP	CD1-CG-CD2	9.06	113.55	106.30
1	A	210	TRP	CD1-CG-CD2	8.95	113.46	106.30
1	A	109	ARG	NE-CZ-NH2	-8.89	115.86	120.30
1	A	51	ARG	NE-CZ-NH1	8.86	124.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	473	LYS	CA-CB-CG	8.84	132.85	113.40
1	A	210	TRP	CG-CD2-CE3	8.72	141.75	133.90
1	A	156	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	A	75	ARG	NE-CZ-NH2	-8.15	116.23	120.30
1	A	437	MET	CG-SD-CE	-8.10	87.24	100.20
1	A	282	TRP	CD1-CG-CD2	7.89	112.61	106.30
1	A	256	TRP	CE2-CD2-CG	-7.86	101.01	107.30
1	A	162	TRP	CE2-CD2-CG	-7.84	101.03	107.30
1	A	216	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	A	35	TRP	CD1-CG-CD2	7.77	112.51	106.30
1	A	35	TRP	CE2-CD2-CG	-7.76	101.09	107.30
1	A	216	ARG	CA-CB-CG	-7.18	97.59	113.40
1	A	259	GLN	CA-CB-CG	7.18	129.20	113.40
1	A	45	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	A	116	TYR	CB-CG-CD2	-7.06	116.77	121.00
1	A	122	TRP	CE2-CD2-CG	-7.04	101.67	107.30
1	A	410	TRP	CE2-CD2-CG	-6.99	101.71	107.30
1	A	29	MET	CG-SD-CE	-6.92	89.13	100.20
1	A	413	ARG	NE-CZ-NH2	-6.85	116.87	120.30
1	A	342	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	410	TRP	CD1-CG-CD2	6.76	111.70	106.30
1	A	210	TRP	CB-CG-CD1	-6.56	118.47	127.00
1	A	366	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	A	109	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	A	366	ARG	O-C-N	-6.48	112.33	122.70
1	A	282	TRP	CE2-CD2-CG	-6.44	102.15	107.30
1	A	344	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	A	344	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	A	26	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	122	TRP	CD1-CG-CD2	6.24	111.29	106.30
1	A	35	TRP	CG-CD2-CE3	6.20	139.48	133.90
1	A	455	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	A	413	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	26	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	A	429	LEU	CA-CB-CG	6.11	129.35	115.30
1	A	208	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	A	29	MET	CA-CB-CG	5.96	123.44	113.30
1	A	256	TRP	CG-CD1-NE1	-5.84	104.26	110.10
1	A	156	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	A	389	VAL	CA-C-N	5.57	129.45	117.20
1	A	255	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	148	LYS	CB-CG-CD	5.54	126.01	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	A	440	ARG	CA-CB-CG	-5.41	101.51	113.40
1	A	360	PRO	CA-C-N	-5.39	105.35	117.20
1	A	270	THR	CA-CB-OG1	-5.34	97.79	109.00
1	A	72	LYS	CA-CB-CG	5.32	125.11	113.40
1	A	162	TRP	CG-CD1-NE1	-5.31	104.79	110.10
1	A	208	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	A	88	MET	N-CA-CB	-5.28	101.10	110.60
1	A	270	THR	N-CA-CB	-5.26	100.31	110.30
1	A	366	ARG	CA-C-N	5.26	128.77	117.20
1	A	270	THR	CA-CB-CG2	5.25	119.75	112.40
1	A	299	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	440	ARG	CB-CG-CD	5.23	125.20	111.60
1	A	369	ALA	N-CA-C	-5.17	97.05	111.00
1	A	271	VAL	N-CA-CB	-5.17	100.14	111.50
1	A	327	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	467	TYR	CB-CG-CD2	-5.12	117.93	121.00
1	A	297	LEU	CB-CG-CD2	-5.11	102.32	111.00
1	A	330	LEU	CB-CG-CD1	-5.06	102.40	111.00
1	A	131	VAL	N-CA-CB	-5.05	100.39	111.50
1	A	210	TRP	CG-CD1-NE1	-5.03	105.07	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	359	CYS	Peptide

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	3861	0	3678	36	0
2	A	43	0	30	1	0
3	A	48	0	26	0	0
4	A	93	0	0	3	0
All	All	4045	0	3734	36	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 5.

All (36) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ASN:HD21	1:A:368:GLY:HA3	1.25	1.01
1:A:348:ASN:ND2	1:A:368:GLY:HA3	1.87	0.89
1:A:131:VAL:HG23	1:A:279:THR:HA	1.65	0.77
1:A:132:PHE:HB3	1:A:278:LEU:HD13	1.66	0.76
1:A:53:OMT:HE3	1:A:144:ASN:HB2	1.73	0.71
1:A:99:ARG:HD2	4:A:518:HOH:O	2.01	0.61
1:A:53:OMT:HE2	1:A:144:ASN:HD22	1.67	0.60
1:A:348:ASN:HD21	1:A:368:GLY:CA	2.08	0.57
1:A:423:ARG:HD3	1:A:463:VAL:O	2.04	0.57
1:A:189:ARG:HD3	1:A:243:ASP:OD2	2.07	0.55
1:A:331:GLN:O	1:A:334:LEU:HB2	2.09	0.53
1:A:239:SER:HB2	4:A:541:HOH:O	2.09	0.52
1:A:426:TYR:OH	1:A:466:GLU:HG3	2.09	0.52
1:A:56:LYS:HE3	1:A:101:ALA:O	2.09	0.52
1:A:96:ALA:O	1:A:148:LYS:HE3	2.11	0.51
1:A:23:ALA:O	1:A:27:GLY:HA3	2.11	0.51
1:A:153:THR:HG22	1:A:155:MET:H	1.75	0.51
1:A:464:HIS:CD2	1:A:466:GLU:HG2	2.45	0.51
1:A:65:THR:HB	1:A:294:TYR:CE1	2.47	0.49
1:A:148:LYS:HE2	4:A:525:HOH:O	2.11	0.49
1:A:398:GLU:HB2	1:A:399:PRO:HD2	1.94	0.49
1:A:464:HIS:HD2	1:A:466:GLU:H	1.60	0.48
1:A:359:CYS:SG	1:A:360:PRO:HD2	2.53	0.48
1:A:371:ARG:HD2	1:A:373:ASP:OD1	2.12	0.48
1:A:173:HIS:O	1:A:177:ILE:HG13	2.14	0.46
1:A:433:GLU:HG2	1:A:437:MET:HE2	1.97	0.46
1:A:267:GLU:O	1:A:270:THR:HB	2.17	0.44
1:A:166:SER:HA	1:A:456:GLN:OE1	2.18	0.44
1:A:399:PRO:HA	1:A:400:PRO:HD3	1.85	0.43
1:A:371:ARG:HA	1:A:371:ARG:HD3	1.90	0.42
1:A:186:LEU:HD23	1:A:190:PHE:CE2	2.56	0.41
1:A:36:PHE:CE1	1:A:40:LEU:HD13	2.56	0.41
1:A:456:GLN:HG3	1:A:460:PHE:CE2	2.56	0.41
1:A:62:GLY:HA3	1:A:296:GLU:O	2.21	0.40
1:A:91:ARG:HD3	2:A:485:HEM:O1D	2.22	0.40
1:A:177:ILE:HG12	1:A:425:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	472/484 (98%)	448 (95%)	20 (4%)	4 (1%)	24	51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	PRO
1	A	196	SER
1	A	366	ARG
1	A	375	ASN

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	407/414 (98%)	376 (92%)	31 (8%)	16	37

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	31	LEU
1	A	40	LEU
1	A	52	ARG
1	A	71	THR
1	A	88	MET
1	A	113	LEU

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Mol	Chain	Res	Type
1	A	152	ARG
1	A	153	THR
1	A	172	LEU
1	A	206	ASN
1	A	237	ARG
1	A	239	SER
1	A	244	LEU
1	A	255	ARG
1	A	262	ILE
1	A	271	VAL
1	A	278	LEU
1	A	281	VAL
1	A	283	PRO
1	A	297	LEU
1	A	306	SER
1	A	318	ILE
1	A	330	LEU
1	A	358	LYS
1	A	359	CYS
1	A	360	PRO
1	A	363	ASN
1	A	366	ARG
1	A	429	LEU
1	A	435	GLN

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

Mol	Chain	Res	Type
1	A	121	ASN
1	A	144	ASN
1	A	145	HIS
1	A	174	GLN
1	A	214	HIS
1	A	300	ASN
1	A	310	GLN
1	A	317	ASN
1	A	348	ASN
1	A	350	HIS
1	A	363	ASN
1	A	464	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	OMT	A	53	1	8,9,10	2.73	3 (37%)	8,12,14	2.14	3 (37%)

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	OMT	A	53	1	-	0/6/8/10	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	OMT	CG-SD	-6.15	1.70	1.78
1	A	53	OMT	CE-SD	-3.48	1.59	1.75
1	A	53	OMT	CB-CA	-2.59	1.51	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	OMT	O-C-CA	-3.12	117.37	125.49
1	A	53	OMT	OD2-SD-OD1	-2.63	109.94	116.85
1	A	53	OMT	OD2-SD-CG	4.11	110.91	108.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	53	OMT	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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	$\# Z > 2$
2	HEM	A	485	1	30,50,50	3.38	11 (36%)	24,82,82	2.27	7 (29%)
3	NDP	A	486	-	42,52,52	1.89	8 (19%)	55,80,80	1.94	15 (27%)

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	485	1	-	0/10/54/54	0/0/8/8
3	NDP	A	486	-	-	0/30/77/77	0/5/5/5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	485	HEM	C3B-C4B	-9.58	1.43	1.51
2	A	485	HEM	C3D-C4D	-6.89	1.42	1.51
2	A	485	HEM	C3B-CAB	-6.85	1.38	1.51
2	A	485	HEM	C2D-C3D	-6.76	1.34	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	485	HEM	C3C-CAC	-6.70	1.38	1.51
3	A	486	NDP	C3B-C2B	-4.48	1.42	1.53
2	A	485	HEM	C2C-C1C	-4.27	1.44	1.52
3	A	486	NDP	C4N-C5N	-4.18	1.40	1.49
3	A	486	NDP	C8A-N7A	-2.45	1.29	1.34
2	A	485	HEM	C2B-C1B	-2.33	1.44	1.51
3	A	486	NDP	C3B-C4B	-2.23	1.47	1.53
2	A	485	HEM	CAD-C3D	-2.15	1.49	1.54
2	A	485	HEM	C2D-C1D	-2.13	1.44	1.51
3	A	486	NDP	O3D-C3D	2.06	1.47	1.43
3	A	486	NDP	O4B-C1B	2.71	1.44	1.41
2	A	485	HEM	CBB-CAB	2.80	1.45	1.29
3	A	486	NDP	C6N-C5N	2.91	1.38	1.33
2	A	485	HEM	CBC-CAC	2.93	1.46	1.29
3	A	486	NDP	O7N-C7N	7.18	1.42	1.24

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	486	NDP	C5B-C4B-C3B	-4.73	96.44	115.21
3	A	486	NDP	O7N-C7N-N7N	-3.59	113.83	122.76
3	A	486	NDP	O4B-C4B-C3B	-3.42	98.26	105.15
3	A	486	NDP	O3D-C3D-C2D	-2.75	102.88	111.83
3	A	486	NDP	O4B-C1B-C2B	-2.19	102.64	106.60
3	A	486	NDP	O3B-C3B-C4B	-2.16	104.56	111.05
3	A	486	NDP	C3B-C2B-C1B	-2.15	98.57	102.73
3	A	486	NDP	C2D-C1D-N1N	-2.05	107.80	113.34
2	A	485	HEM	CAA-CBA-CGA	2.01	116.44	112.75
3	A	486	NDP	O4D-C4D-C3D	2.11	109.40	105.15
3	A	486	NDP	O2X-P2B-O1X	2.42	118.38	110.58
3	A	486	NDP	C5N-C4N-C3N	2.50	119.40	112.52
2	A	485	HEM	CMD-C2D-C3D	2.67	126.17	114.35
2	A	485	HEM	C2D-C3D-C4D	3.05	106.67	101.50
3	A	486	NDP	P2B-O2B-C2B	3.06	128.90	121.56
3	A	486	NDP	O4B-C1B-N9A	3.59	115.61	108.10
2	A	485	HEM	CAD-C3D-C4D	3.78	125.79	112.47
3	A	486	NDP	O2B-C2B-C3B	4.13	127.59	111.51
2	A	485	HEM	CMC-C2C-C3C	4.47	127.70	116.53
2	A	485	HEM	CAD-C3D-C2D	4.96	127.48	113.22
3	A	486	NDP	C2B-C3B-C4B	5.60	115.11	101.85
2	A	485	HEM	CMB-C2B-C3B	6.00	131.52	116.53

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
2	A	485	HEM	1	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 [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	474/484 (97%)	-1.06	1 (0%) 95 96	10, 26, 47, 76	8 (1%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	360	PRO	3.0

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	OMT	A	53	10/11	0.99	0.05	-	14,18,25,26	0

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(\AA^2)	Q<0.9
2	HEM	A	485	43/43	0.99	0.07	-0.44	4,15,21,24	0
3	NDP	A	486	48/48	0.98	0.08	-0.55	22,29,37,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.