



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:17 AM EDT

PDB ID : 2CAH / pdb_00002cah
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

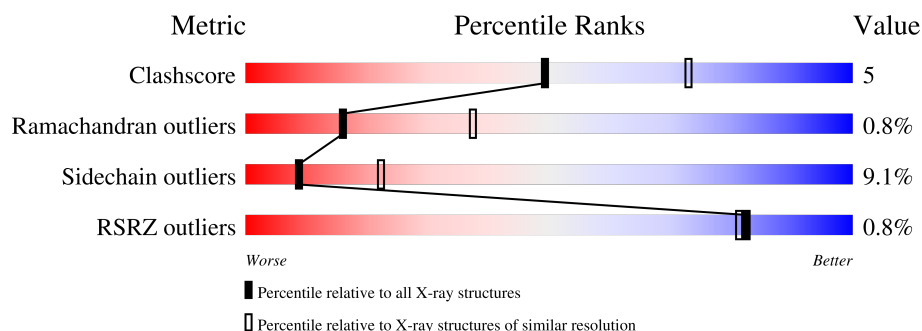
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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	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 (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



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

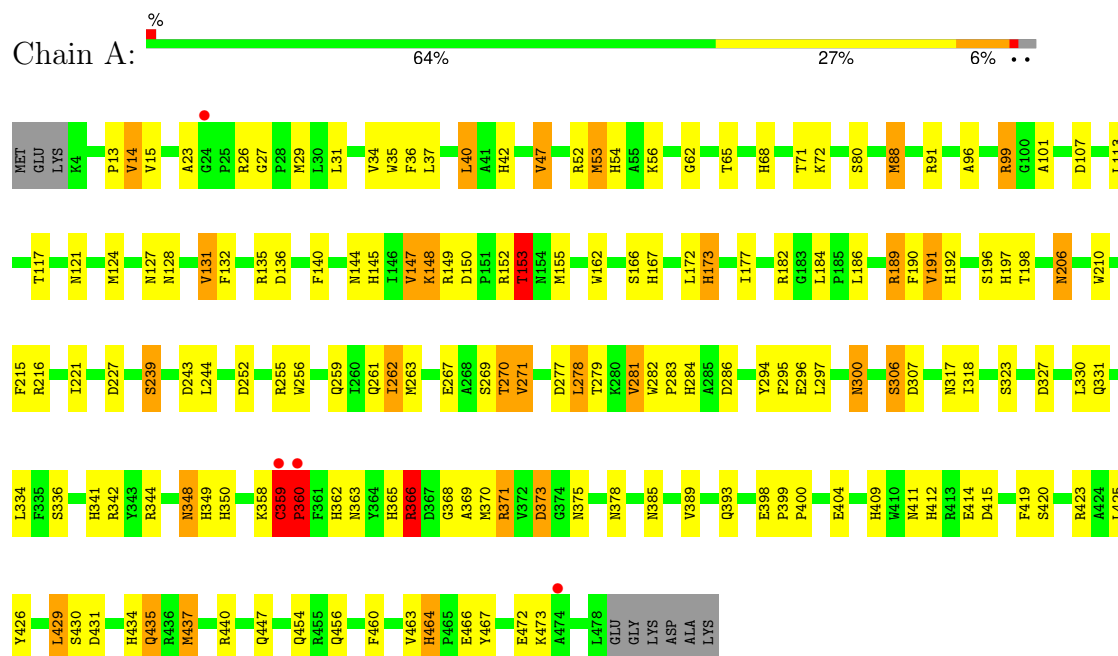
- Molecule 4 is water.

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

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



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 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.0 (15.00-2.70) 90.3 (15.00-2.70)	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) 0.178 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
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 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 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: 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	1.16	24/3961 (0.6%)	1.91	131/5359 (2.4%)

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

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	HIS	CD2-NE2	-7.45	1.29	1.37
1	A	412	HIS	CD2-NE2	-7.33	1.29	1.37
1	A	197	HIS	CD2-NE2	-6.98	1.30	1.37
1	A	54	HIS	CD2-NE2	-6.90	1.30	1.37
1	A	284	HIS	CD2-NE2	-6.81	1.30	1.37
1	A	145	HIS	CD2-NE2	-6.67	1.30	1.37
1	A	192	HIS	CD2-NE2	-6.67	1.30	1.37
1	A	349	HIS	CD2-NE2	-6.64	1.30	1.37
1	A	47	VAL	CA-CB	6.62	1.62	1.54
1	A	350	HIS	CD2-NE2	-6.47	1.30	1.37
1	A	362	HIS	CD2-NE2	-6.43	1.30	1.37
1	A	434	HIS	CD2-NE2	-6.20	1.31	1.37
1	A	464	HIS	CD2-NE2	-6.11	1.31	1.37
1	A	341	HIS	CD2-NE2	-6.11	1.31	1.37
1	A	117	THR	CA-CB	6.07	1.63	1.53
1	A	323	SER	CA-CB	-5.96	1.45	1.53
1	A	167	HIS	CG-ND1	-5.84	1.31	1.38
1	A	365	HIS	CD2-NE2	-5.49	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	349	HIS	CG-ND1	-5.35	1.32	1.38
1	A	68	HIS	CD2-NE2	-5.34	1.31	1.37
1	A	173	HIS	CD2-NE2	-5.33	1.31	1.37
1	A	409	HIS	CD2-NE2	-5.31	1.32	1.37
1	A	434	HIS	CG-ND1	-5.07	1.32	1.38
1	A	284	HIS	CG-ND1	-5.03	1.32	1.38

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	369	ALA	N-CA-C	-11.94	97.05	112.93
1	A	131	VAL	N-CA-CB	-10.37	100.39	112.32
1	A	473	LYS	CA-CB-CG	9.38	132.85	114.10
1	A	295	PHE	CA-CB-CG	9.04	122.84	113.80
1	A	127	ASN	OD1-CG-ND2	-8.88	113.72	122.60
1	A	371	ARG	NE-CZ-NH1	8.74	130.24	121.50
1	A	348	ASN	CA-CB-CG	-8.46	104.14	112.60
1	A	348	ASN	OD1-CG-ND2	-8.39	114.20	122.60
1	A	216	ARG	CA-CB-CG	-8.25	97.59	114.10
1	A	373	ASP	CA-CB-CG	8.11	120.71	112.60
1	A	412	HIS	CB-CG-CD2	-7.92	120.90	131.20
1	A	271	VAL	N-CA-CB	-7.91	100.14	111.21
1	A	270	THR	CA-CB-OG1	-7.88	97.79	109.60
1	A	197	HIS	CB-CG-CD2	-7.86	120.98	131.20
1	A	362	HIS	CB-CG-CD2	-7.86	120.99	131.20
1	A	210	TRP	CG-CD2-CE3	7.85	141.75	133.90
1	A	366	ARG	O-C-N	-7.72	112.33	122.59
1	A	259	GLN	CA-CB-CG	7.55	129.20	114.10
1	A	472	GLU	CA-C-N	7.52	130.36	120.28
1	A	472	GLU	C-N-CA	7.52	130.36	120.28
1	A	336	SER	N-CA-C	7.52	119.47	111.28
1	A	371	ARG	NE-CZ-NH2	-7.41	112.53	119.20
1	A	363	ASN	OD1-CG-ND2	-7.39	115.21	122.60
1	A	259	GLN	OE1-CD-NE2	-7.27	115.33	122.60
1	A	317	ASN	OD1-CG-ND2	-7.13	115.47	122.60
1	A	409	HIS	CB-CG-CD2	-7.12	121.94	131.20
1	A	80	SER	N-CA-C	7.02	120.94	112.38
1	A	131	VAL	CG1-CB-CG2	-6.99	95.41	110.80
1	A	150	ASP	CA-CB-CG	6.85	119.45	112.60
1	A	148	LYS	O-C-N	-6.74	116.41	121.47
1	A	300	ASN	OD1-CG-ND2	-6.70	115.90	122.60
1	A	252	ASP	CA-CB-CG	6.70	119.30	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	VAL	N-CA-CB	-6.67	101.26	112.47
1	A	414	GLU	N-CA-C	-6.67	103.83	112.23
1	A	107	ASP	CA-CB-CG	6.63	119.23	112.60
1	A	378	ASN	OD1-CG-ND2	-6.61	116.00	122.60
1	A	26	ARG	N-CA-CB	-6.54	102.05	111.54
1	A	270	THR	N-CA-CB	-6.49	100.31	110.30
1	A	327	ASP	CA-CB-CG	6.47	119.07	112.60
1	A	148	LYS	CB-CG-CD	6.40	126.01	111.30
1	A	131	VAL	O-C-N	-6.39	115.98	122.75
1	A	88	MET	N-CA-CB	-6.33	101.10	111.66
1	A	221	ILE	N-CA-C	-6.32	98.42	107.77
1	A	440	ARG	CA-CB-CG	-6.30	101.51	114.10
1	A	359	CYS	CA-C-N	6.29	127.70	119.84
1	A	359	CYS	C-N-CA	6.29	127.70	119.84
1	A	393	GLN	CA-C-N	6.29	126.41	119.87
1	A	393	GLN	C-N-CA	6.29	126.41	119.87
1	A	269	SER	CA-C-N	6.24	131.28	120.68
1	A	269	SER	C-N-CA	6.24	131.28	120.68
1	A	437	MET	CG-SD-CE	-6.21	87.24	100.90
1	A	191	VAL	N-CA-CB	-6.18	101.23	111.36
1	A	192	HIS	CB-CG-CD2	-6.14	123.21	131.20
1	A	270	THR	N-CA-C	6.12	119.94	112.23
1	A	385	ASN	OD1-CG-ND2	-6.10	116.50	122.60
1	A	210	TRP	CE2-CD2-CG	-6.08	99.91	107.20
1	A	440	ARG	CB-CG-CD	6.04	125.20	111.30
1	A	153	THR	CA-CB-OG1	-6.00	100.60	109.60
1	A	286	ASP	CA-CB-CG	6.00	118.60	112.60
1	A	415	ASP	N-CA-C	-6.00	99.37	108.67
1	A	362	HIS	CB-CG-ND1	5.99	131.68	122.70
1	A	389	VAL	O-C-N	-5.92	115.17	122.57
1	A	431	ASP	CA-CB-CG	-5.89	106.71	112.60
1	A	420	SER	N-CA-C	5.83	117.31	111.07
1	A	262	ILE	CB-CG1-CD1	-5.77	101.69	113.80
1	A	13	PRO	CA-C-N	-5.76	115.53	122.90
1	A	13	PRO	C-N-CA	-5.76	115.53	122.90
1	A	435	GLN	OE1-CD-NE2	-5.75	116.85	122.60
1	A	68	HIS	CA-CB-CG	-5.72	108.08	113.80
1	A	15	VAL	N-CA-C	5.71	115.90	110.53
1	A	307	ASP	CA-CB-CG	5.71	118.31	112.60
1	A	366	ARG	CA-C-N	-5.70	114.70	123.14
1	A	366	ARG	C-N-CA	-5.70	114.70	123.14
1	A	454	GLN	OE1-CD-NE2	-5.68	116.92	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	ARG	CA-CB-CG	-5.67	102.75	114.10
1	A	198	THR	N-CA-C	-5.66	99.97	108.96
1	A	360	PRO	O-C-N	5.63	130.24	122.64
1	A	210	TRP	CB-CG-CD1	-5.62	118.47	126.90
1	A	467	TYR	N-CA-C	-5.59	104.58	111.40
1	A	306	SER	CA-CB-OG	5.59	122.28	111.10
1	A	35	TRP	CG-CD2-CE3	5.58	139.48	133.90
1	A	371	ARG	CA-C-O	5.57	126.71	120.92
1	A	473	LYS	N-CA-CB	-5.52	102.01	110.12
1	A	72	LYS	CA-CB-CG	5.50	125.11	114.10
1	A	227	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	131	VAL	CB-CA-C	5.48	118.91	110.91
1	A	128	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	A	261	GLN	N-CA-C	-5.46	100.00	108.90
1	A	153	THR	N-CA-CB	-5.45	101.52	110.40
1	A	149	ARG	N-CA-C	5.44	118.61	109.95
1	A	270	THR	CA-CB-CG2	5.44	119.75	110.50
1	A	341	HIS	CB-CG-CD2	-5.42	124.16	131.20
1	A	121	ASN	CB-CG-ND2	5.42	124.52	116.40
1	A	440	ARG	NE-CZ-NH2	-5.41	114.33	119.20
1	A	29	MET	CG-SD-CE	-5.35	89.13	100.90
1	A	350	HIS	CB-CG-CD2	-5.35	124.25	131.20
1	A	360	PRO	CA-N-CD	-5.34	104.52	112.00
1	A	147	VAL	CB-CA-C	5.33	119.17	111.65
1	A	419	PHE	N-CA-C	5.32	121.17	114.31
1	A	369	ALA	CA-C-N	-5.31	115.67	122.79
1	A	369	ALA	C-N-CA	-5.31	115.67	122.79
1	A	263	MET	CA-C-N	5.30	125.06	119.76
1	A	263	MET	C-N-CA	5.30	125.06	119.76
1	A	29	MET	CB-CA-C	-5.28	100.61	109.53
1	A	42	HIS	CB-CG-CD2	-5.26	124.37	131.20
1	A	34	VAL	N-CA-C	5.23	117.62	111.09
1	A	121	ASN	OD1-CG-ND2	-5.21	117.39	122.60
1	A	206	ASN	CB-CG-ND2	5.20	124.19	116.40
1	A	136	ASP	CA-C-N	5.17	124.78	119.56
1	A	136	ASP	C-N-CA	5.17	124.78	119.56
1	A	447	GLN	OE1-CD-NE2	-5.16	117.44	122.60
1	A	184	LEU	CA-C-N	5.16	125.44	119.92
1	A	184	LEU	C-N-CA	5.16	125.44	119.92
1	A	256	TRP	CE2-CD2-CG	-5.16	101.01	107.20
1	A	162	TRP	CE2-CD2-CG	-5.14	101.03	107.20
1	A	99	ARG	N-CA-C	5.14	121.75	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	HIS	CB-CG-ND1	5.13	130.40	122.70
1	A	277	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	464	HIS	N-CA-C	-5.11	98.51	109.81
1	A	35	TRP	CE2-CD2-CG	-5.09	101.09	107.20
1	A	167	HIS	CB-CG-CD2	-5.08	124.60	131.20
1	A	411	ASN	OD1-CG-ND2	-5.07	117.53	122.60
1	A	189	ARG	NE-CZ-NH1	5.06	126.56	121.50
1	A	344	ARG	N-CA-CB	-5.06	102.69	110.12
1	A	430	SER	N-CA-C	5.05	116.62	110.41
1	A	365	HIS	CA-CB-CG	-5.05	108.75	113.80
1	A	14	VAL	CA-C-O	5.05	126.09	120.59
1	A	42	HIS	CB-CG-ND1	5.04	130.26	122.70
1	A	282	TRP	CB-CA-C	-5.03	105.19	110.17
1	A	409	HIS	CB-CG-ND1	5.01	130.22	122.70
1	A	128	ASN	CA-CB-CG	5.00	117.61	112.60

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	41	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	41	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 (41) 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:53:OMT:HE1	1:A:144:ASN:HB2	1.61	0.83
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:429:LEU:HD23	1:A:437:MET:HE1	1.76	0.68
1:A:99:ARG:HD2	4:A:518:HOH:O	2.01	0.61
1:A:53:OMT:HE2	1:A:140:PHE:CE2	2.36	0.61
1:A:153:THR:HG23	1:A:155:MET:HE3	1.85	0.59
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:124:MET:HE2	1:A:215:PHE:CE1	2.45	0.52
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:429:LEU:CD2	1:A:437:MET:HE1	2.43	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:HD3	1:A:371:ARG:HA	1.90	0.42
1:A:36:PHE:CE1	1:A:40:LEU:HD13	2.56	0.41
1:A:186:LEU:HD23	1:A:190:PHE:CE2	2.56	0.41
1:A:370:MET:HE2	1:A:370:MET:HB2	1.97	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:53:OMT:CE	1:A:144:ASN:HD22	2.35	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%)	16	37

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%)	370 (91%)	37 (9%)	9	22

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	31	LEU
1	A	37	LEU
1	A	40	LEU
1	A	47	VAL
1	A	52	ARG
1	A	71	THR

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Mol	Chain	Res	Type
1	A	88	MET
1	A	113	LEU
1	A	135	ARG
1	A	147	VAL
1	A	152	ARG
1	A	153	THR
1	A	172	LEU
1	A	182	ARG
1	A	191	VAL
1	A	206	ASN
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	300	ASN
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	366	ARG
1	A	404	GLU
1	A	429	LEU
1	A	435	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
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	317	ASN

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Mol	Chain	Res	Type
1	A	331	GLN
1	A	348	ASN
1	A	350	HIS
1	A	363	ASN
1	A	378	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	2.94	2 (25%)	6,12,14	2.28	2 (33%)

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	-	1/7/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	OMT	CG-SD	-6.13	1.70	1.78
1	A	53	OMT	CE-SD	-4.99	1.59	1.75

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	OMT	OD2-SD-OD1	-3.88	109.94	117.22
1	A	53	OMT	OD2-SD-CG	3.59	110.91	108.33

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	53	OMT	CB-CG-SD-CE

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	53	OMT	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
3	NDP	A	486	-	51,52,52	1.88	5 (9%)	71,80,80	1.97	17 (23%)
2	HEM	A	485	1	50,50,50	1.37	6 (12%)	67,82,82	1.04	3 (4%)

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
3	NDP	A	486	-	-	9/34/77/77	0/5/5/5
2	HEM	A	485	1	-	2/14/54/54	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	486	NDP	O7N-C7N	7.70	1.42	1.24
3	A	486	NDP	C4N-C3N	-5.75	1.39	1.50
3	A	486	NDP	C3B-C2B	-4.62	1.42	1.53
3	A	486	NDP	C4N-C5N	-3.46	1.40	1.49
2	A	485	HEM	CAB-C3B	-3.34	1.38	1.47
2	A	485	HEM	CBC-CAC	3.30	1.46	1.30
2	A	485	HEM	CAC-C3C	-3.23	1.38	1.47
2	A	485	HEM	CBB-CAB	3.14	1.45	1.30
2	A	485	HEM	O2A-CGA	-2.59	1.22	1.30
3	A	486	NDP	C3B-C4B	-2.36	1.47	1.53
2	A	485	HEM	O2D-CGD	-2.31	1.23	1.30

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	486	NDP	C3N-C7N-N7N	6.15	128.59	117.67
3	A	486	NDP	C2B-C3B-C4B	6.10	115.11	101.99
3	A	486	NDP	C5B-C4B-C3B	-5.21	96.44	115.21
3	A	486	NDP	O2B-C2B-C3B	4.44	127.59	111.68
3	A	486	NDP	O7N-C7N-N7N	-4.04	113.83	122.89
3	A	486	NDP	O4B-C1B-N9A	3.92	115.61	108.09
3	A	486	NDP	C2B-C1B-N9A	3.91	120.18	113.75
3	A	486	NDP	O4B-C4B-C3B	-3.47	98.26	105.15
2	A	485	HEM	C3B-C4B-NB	2.88	111.54	109.47
3	A	486	NDP	O3D-C3D-C2D	-2.79	102.88	111.82
3	A	486	NDP	O4B-C1B-C2B	-2.29	102.64	106.59
3	A	486	NDP	O3B-C3B-C4B	-2.27	104.56	111.08
3	A	486	NDP	C2D-C1D-N1N	-2.24	107.80	113.31
3	A	486	NDP	O2A-PA-O3	2.22	113.28	107.27
3	A	486	NDP	C3B-C2B-C1B	-2.21	98.57	102.81
3	A	486	NDP	O4D-C4D-C3D	2.14	109.40	105.15
2	A	485	HEM	O2A-CGA-CBA	2.13	120.73	114.00
2	A	485	HEM	CAD-CBD-CGD	-2.07	108.17	113.67
3	A	486	NDP	P2B-O2B-C2B	2.05	128.90	123.43
3	A	486	NDP	O4D-C1D-C2D	2.00	110.90	106.62

There are no chirality outliers.

All (11) torsion outliers are listed below:

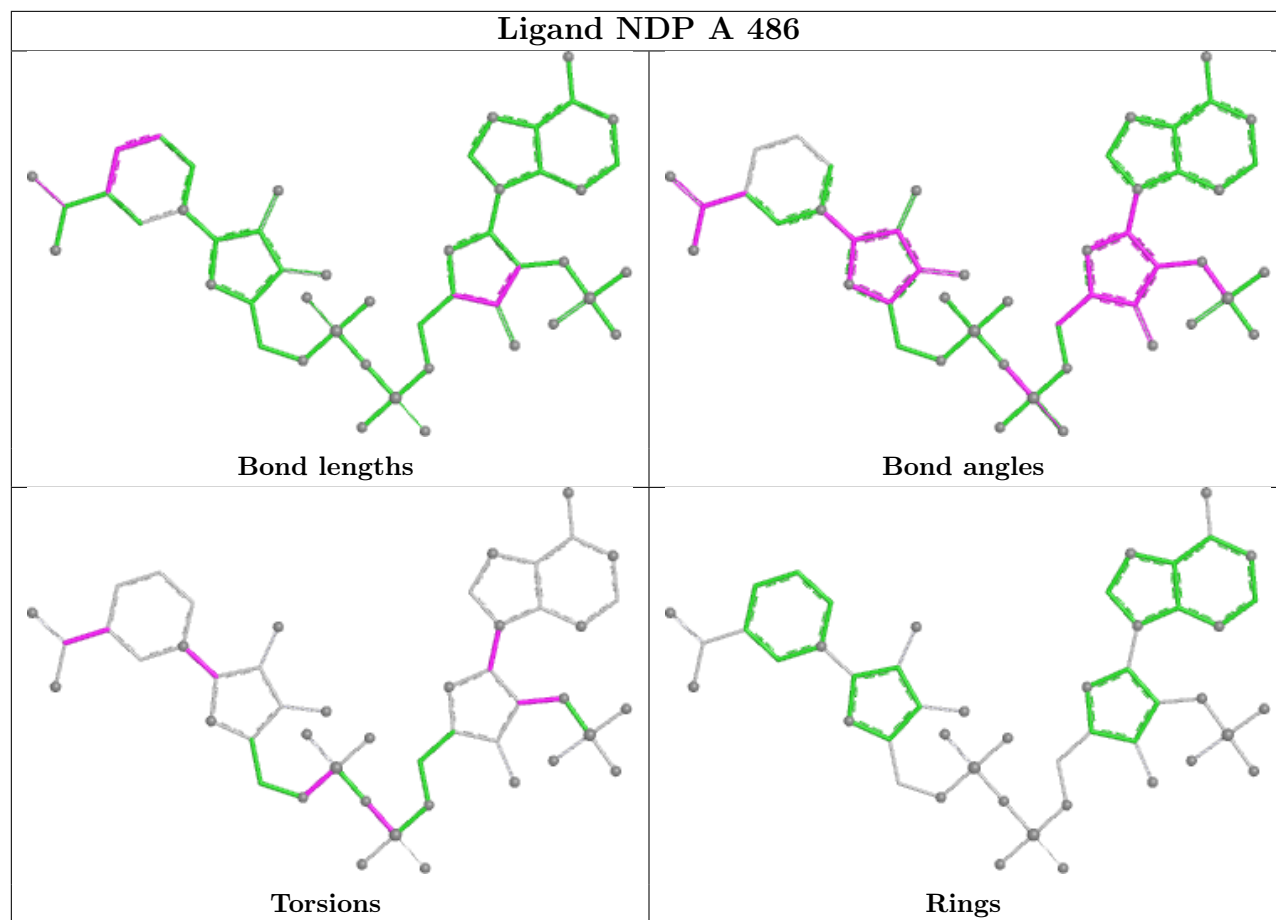
Mol	Chain	Res	Type	Atoms
3	A	486	NDP	C1B-C2B-O2B-P2B
3	A	486	NDP	C3B-C2B-O2B-P2B
3	A	486	NDP	O4D-C1D-N1N-C6N
3	A	486	NDP	C5D-O5D-PN-O1N
3	A	486	NDP	PN-O3-PA-O2A
2	A	485	HEM	CAD-CBD-CGD-O2D
2	A	485	HEM	CAD-CBD-CGD-O1D
3	A	486	NDP	C2N-C3N-C7N-N7N
3	A	486	NDP	PN-O3-PA-O1A
3	A	486	NDP	O4B-C1B-N9A-C8A
3	A	486	NDP	C2B-C1B-N9A-C8A

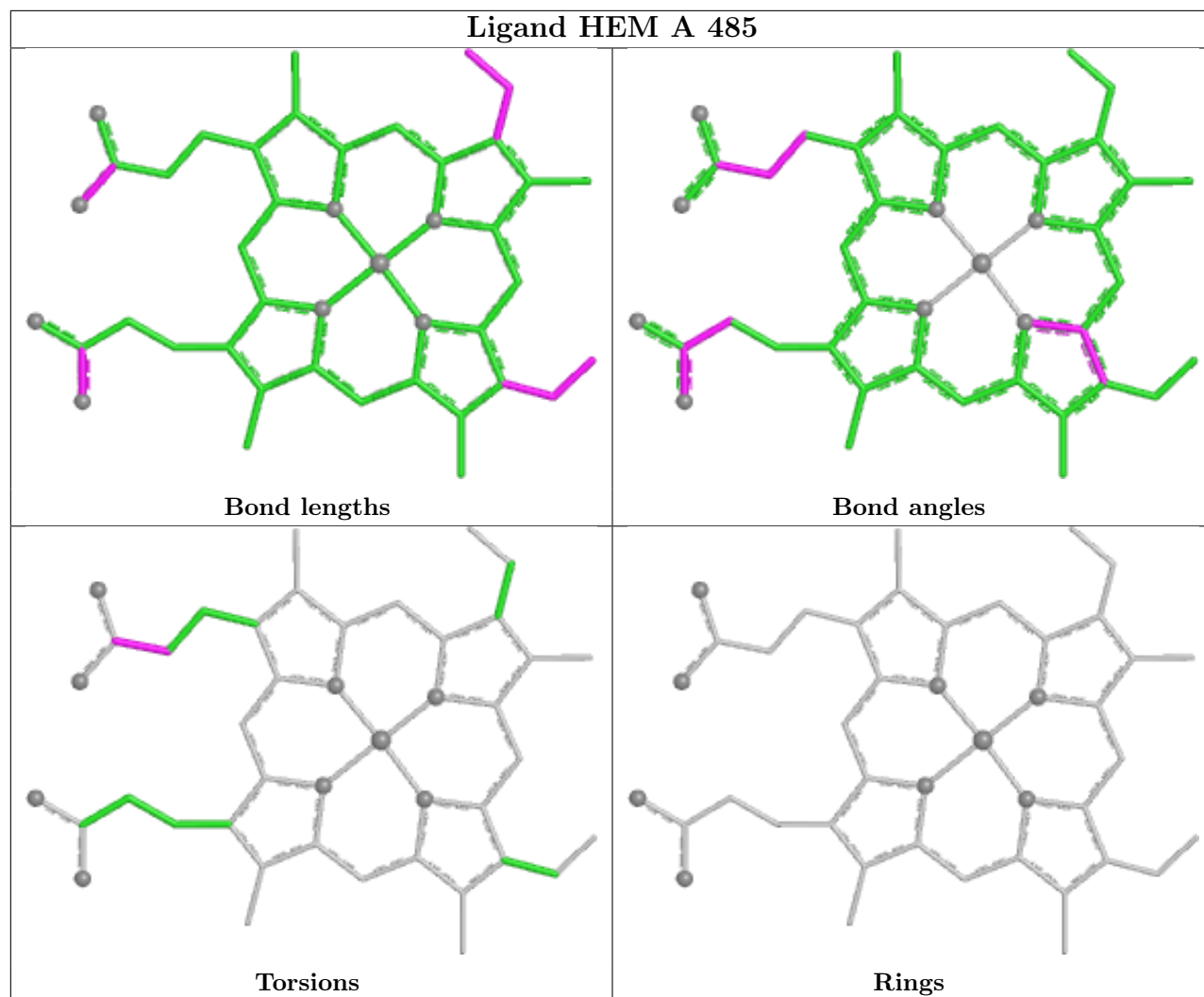
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	485	HEM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	474/484 (97%)	-0.46	4 (0%) 82 81	10, 26, 47, 76	8 (1%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	359	CYS	3.6
1	A	360	PRO	2.7
1	A	24	GLY	2.2
1	A	474	ALA	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	OMT	A	53	10/11	0.98	0.06	14,18,25,26	0

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

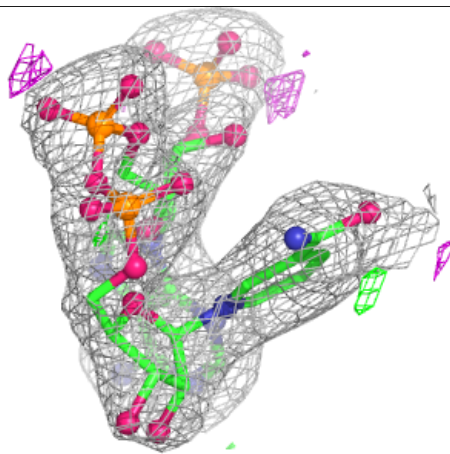
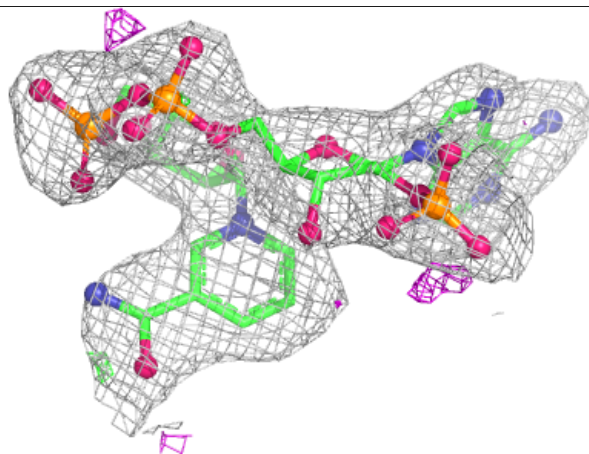
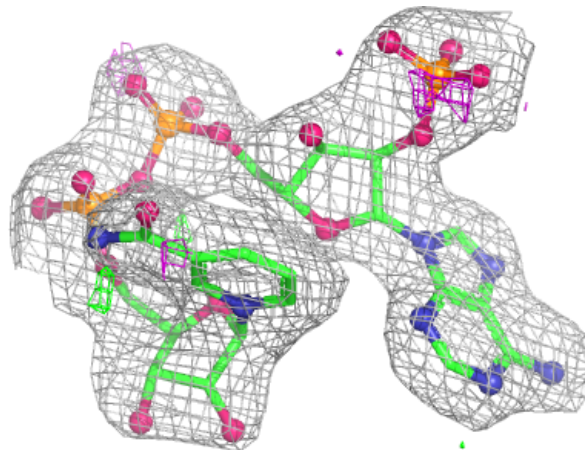
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

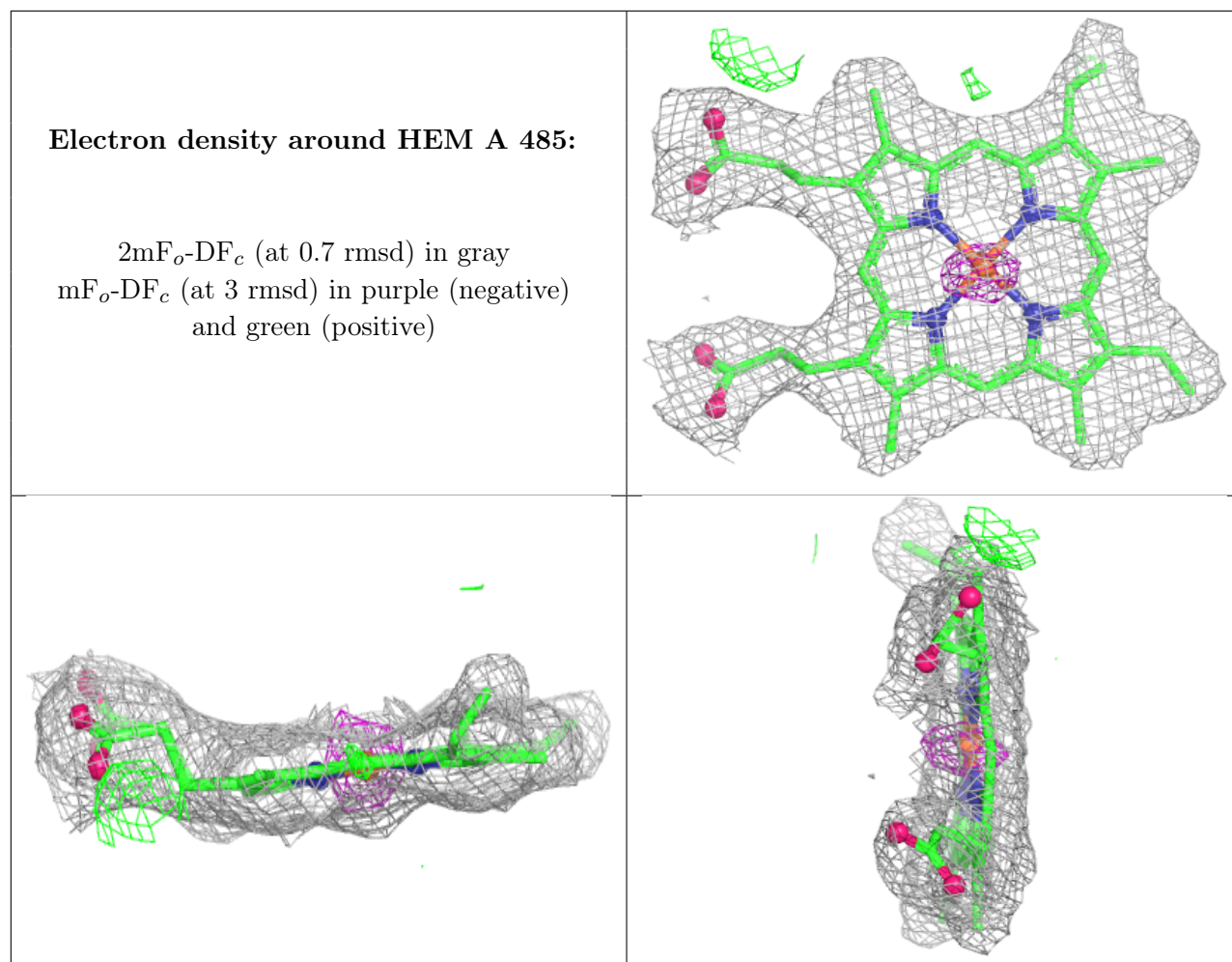
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NDP	A	486	48/48	0.96	0.07	22,29,37,42	0
2	HEM	A	485	43/43	0.98	0.06	4,15,21,24	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NDP A 486:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.