WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2023 – 07:54 PM EDT

PDB ID	:	4E37
Title	:	Crystal Structure of P. aeruginosa catalase, KatA tetramer
Authors	:	VanderWielen, B.D.; Wilson, J.J.; Kovall, R.A.
Deposited on	:	2012-03-09
Resolution	:	2.53 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:

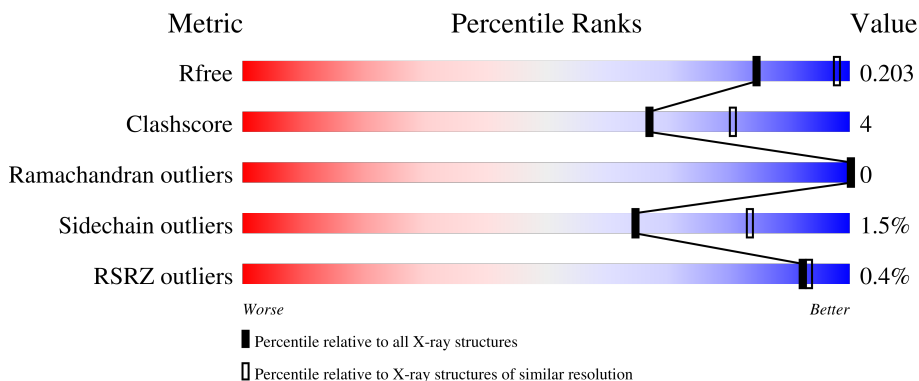|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.53 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	Percentile Ranks	Value
Rfree		0.203
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		1.5%
RSRZ outliers		0.4%

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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 <=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	88% · · · 10% · ·
1	B	484	89% · · · 10% · ·
1	C	484	% · 87% · · · 10% · ·
1	D	484	88% · · · 10% · ·

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 16548 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	479	Total 3915	C 2485	N 704	O 717	S 9	0	0	0
1	B	480	Total 3923	C 2489	N 705	O 720	S 9	0	0	0
1	C	479	Total 3928	C 2493	N 708	O 718	S 9	0	2	0
1	D	480	Total 3932	C 2494	N 707	O 722	S 9	0	1	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	483	ALA	-	expression tag	UNP O52762
A	484	ALA	-	expression tag	UNP O52762
A	485	HIS	-	expression tag	UNP O52762
A	486	HIS	-	expression tag	UNP O52762
B	483	ALA	-	expression tag	UNP O52762
B	484	ALA	-	expression tag	UNP O52762
B	485	HIS	-	expression tag	UNP O52762
B	486	HIS	-	expression tag	UNP O52762
C	483	ALA	-	expression tag	UNP O52762
C	484	ALA	-	expression tag	UNP O52762
C	485	HIS	-	expression tag	UNP O52762
C	486	HIS	-	expression tag	UNP O52762
D	483	ALA	-	expression tag	UNP O52762
D	484	ALA	-	expression tag	UNP O52762
D	485	HIS	-	expression tag	UNP O52762
D	486	HIS	-	expression tag	UNP O52762

- 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		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	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: $C_{21}H_{30}N_7O_{17}P_3$).
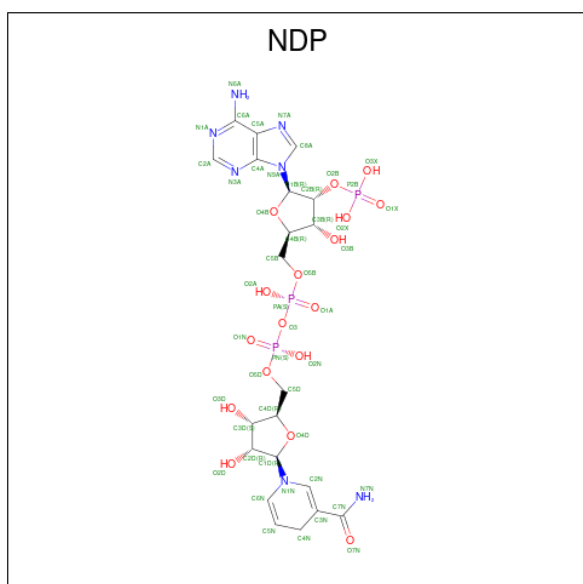
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	D	1	Total 48	C 21	N 7	O 17	P 3	0	0

• Molecule 4 is water.

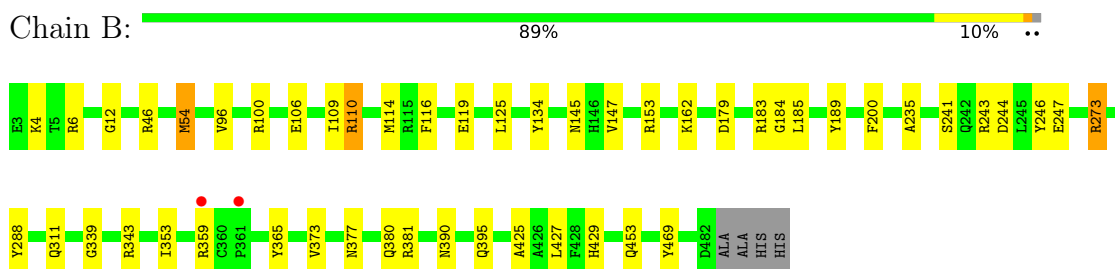| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	130	Total 130	O 130	0	0
4	B	136	Total 136	O 136	0	0
4	C	116	Total 116	O 116	0	0
4	D	104	Total 104	O 104	0	0

3 Residue-property plots ⓘ

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.
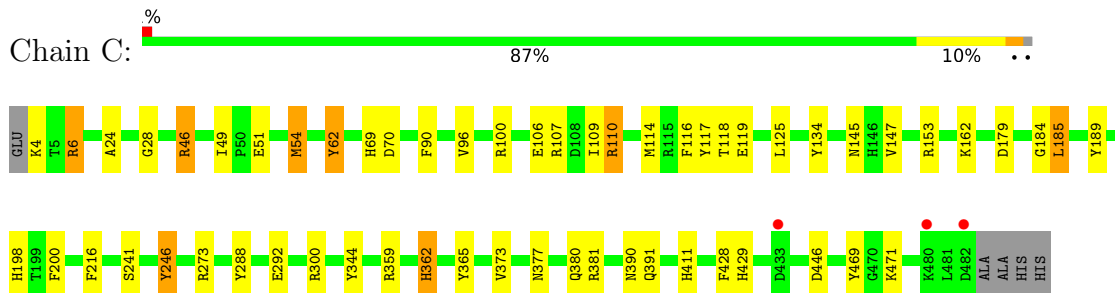
• Molecule 1: Catalase
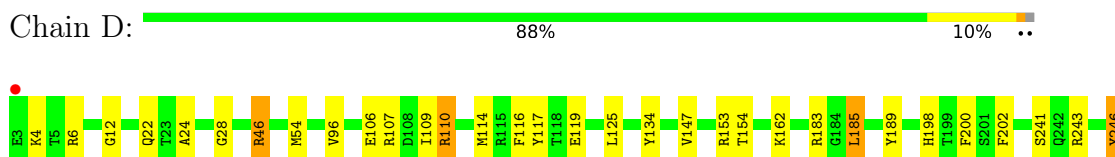
Chain A:

• Molecule 1: Catalase

Chain B:

• Molecule 1: Catalase

Chain C:

• Molecule 1: Catalase

Chain D:

E247 E250 R273 Y288 Q311 Y344 I353 R359 Y365 V373 N377 Q380 R381 N390 F428 H429 L430 F431 K436 R457 Y469 D482 ALA ALA HIS HIS
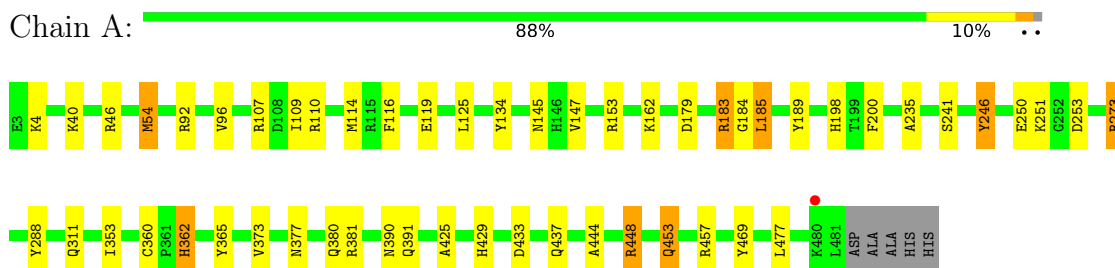
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.73Å 167.43Å 90.55Å 90.00° 111.40° 90.00°	Depositor
Resolution (Å)	43.46 – 2.53 43.46 – 2.53	Depositor EDS
% Data completeness (in resolution range)	98.6 (43.46-2.53) 98.6 (43.46-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	5.04 (at 2.54Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_918)	Depositor
R, R_{free}	0.174 , 0.201 0.177 , 0.203	Depositor DCC
R_{free} test set	3107 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	25.2	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 19.5	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16548	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: OMT, HEM, NDP

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	0.77	14/4020 (0.3%)	0.75	16/5453 (0.3%)
1	B	1.01	19/4028 (0.5%)	0.77	24/5464 (0.4%)
1	C	1.11	25/4039 (0.6%)	0.87	33/5478 (0.6%)
1	D	0.92	17/4037 (0.4%)	0.75	18/5476 (0.3%)
All	All	0.96	75/16124 (0.5%)	0.79	91/21871 (0.4%)

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	134	TYR	CE1-CZ	-21.53	1.10	1.38
1	B	134	TYR	CE2-CZ	-20.72	1.11	1.38
1	C	288	TYR	CE1-CZ	-19.54	1.13	1.38
1	C	288	TYR	CE2-CZ	-18.86	1.14	1.38
1	D	365	TYR	CE1-CZ	-18.62	1.14	1.38
1	B	134	TYR	CG-CD1	-18.39	1.15	1.39
1	D	365	TYR	CE2-CZ	-18.39	1.14	1.38
1	B	134	TYR	CG-CD2	-18.36	1.15	1.39
1	C	288	TYR	CG-CD2	-17.29	1.16	1.39
1	C	288	TYR	CG-CD1	-17.23	1.16	1.39
1	D	365	TYR	CG-CD1	-16.52	1.17	1.39
1	C	62	TYR	CE2-CZ	-16.32	1.17	1.38
1	D	365	TYR	CG-CD2	-16.18	1.18	1.39
1	C	62	TYR	CE1-CZ	-16.15	1.17	1.38
1	C	216	PHE	CG-CD2	-14.60	1.16	1.38
1	C	216	PHE	CG-CD1	-14.60	1.16	1.38
1	C	62	TYR	CG-CD1	-14.23	1.20	1.39
1	C	62	TYR	CG-CD2	-13.99	1.21	1.39
1	A	246	TYR	CE2-CZ	-13.04	1.21	1.38
1	D	246	TYR	CE1-CZ	-13.02	1.21	1.38
1	D	246	TYR	CE2-CZ	-13.01	1.21	1.38
1	B	246	TYR	CE2-CZ	-13.00	1.21	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	200	PHE	CG-CD1	-12.76	1.19	1.38
1	B	200	PHE	CG-CD2	-12.72	1.19	1.38
1	B	246	TYR	CE1-CZ	-12.70	1.22	1.38
1	A	246	TYR	CE1-CZ	-12.69	1.22	1.38
1	C	246	TYR	CE1-CZ	-12.64	1.22	1.38
1	C	246	TYR	CE2-CZ	-12.28	1.22	1.38
1	A	246	TYR	CG-CD1	-11.41	1.24	1.39
1	C	216	PHE	CE2-CZ	-11.25	1.16	1.37
1	A	246	TYR	CG-CD2	-11.10	1.24	1.39
1	B	246	TYR	CG-CD1	-11.05	1.24	1.39
1	C	246	TYR	CG-CD1	-10.93	1.25	1.39
1	D	246	TYR	CG-CD1	-10.87	1.25	1.39
1	D	246	TYR	CG-CD2	-10.80	1.25	1.39
1	C	246	TYR	CG-CD2	-10.37	1.25	1.39
1	C	216	PHE	CE1-CZ	-10.30	1.17	1.37
1	B	200	PHE	CE1-CZ	-10.18	1.18	1.37
1	B	246	TYR	CG-CD2	-10.13	1.25	1.39
1	B	200	PHE	CE2-CZ	-10.12	1.18	1.37
1	D	116	PHE	CG-CD2	-9.59	1.24	1.38
1	C	116	PHE	CG-CD1	-8.96	1.25	1.38
1	D	116	PHE	CG-CD1	-8.94	1.25	1.38
1	A	116	PHE	CG-CD1	-8.94	1.25	1.38
1	B	116	PHE	CG-CD2	-8.66	1.25	1.38
1	A	116	PHE	CG-CD2	-8.65	1.25	1.38
1	C	116	PHE	CG-CD2	-8.56	1.25	1.38
1	B	116	PHE	CG-CD1	-8.48	1.26	1.38
1	A	134	TYR	CE2-CZ	-6.91	1.29	1.38
1	D	134	TYR	CE2-CZ	-6.72	1.29	1.38
1	D	116	PHE	CE1-CZ	-6.66	1.24	1.37
1	C	134	TYR	CE2-CZ	-6.54	1.30	1.38
1	A	288	TYR	CE1-CZ	-6.50	1.30	1.38
1	A	134	TYR	CE1-CZ	-6.50	1.30	1.38
1	A	116	PHE	CE2-CZ	-6.18	1.25	1.37
1	D	288	TYR	CE1-CZ	-6.11	1.30	1.38
1	C	116	PHE	CE2-CZ	-6.02	1.25	1.37
1	C	116	PHE	CE1-CZ	-5.85	1.26	1.37
1	C	365	TYR	CE1-CZ	-5.79	1.31	1.38
1	B	288	TYR	CE2-CZ	-5.63	1.31	1.38
1	D	116	PHE	CE2-CZ	-5.53	1.26	1.37
1	A	134	TYR	CG-CD2	-5.39	1.32	1.39
1	A	288	TYR	CE2-CZ	-5.39	1.31	1.38
1	B	116	PHE	CE2-CZ	-5.38	1.27	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	288	TYR	CE2-CZ	-5.37	1.31	1.38
1	B	288	TYR	CE1-CZ	-5.32	1.31	1.38
1	C	365	TYR	CE2-CZ	-5.30	1.31	1.38
1	D	134	TYR	CG-CD1	-5.28	1.32	1.39
1	B	116	PHE	CE1-CZ	-5.26	1.27	1.37
1	D	134	TYR	CE1-CZ	-5.26	1.31	1.38
1	B	365	TYR	CE1-CZ	-5.26	1.31	1.38
1	C	134	TYR	CE1-CZ	-5.16	1.31	1.38
1	A	116	PHE	CE1-CZ	-5.13	1.27	1.37
1	A	365	TYR	CE2-CZ	-5.05	1.31	1.38
1	C	134	TYR	CG-CD2	-5.02	1.32	1.39

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	6	ARG	NE-CZ-NH1	-15.48	112.56	120.30
1	C	6	ARG	NE-CZ-NH2	15.37	127.99	120.30
1	C	46	ARG	NE-CZ-NH2	13.32	126.96	120.30
1	C	46	ARG	NE-CZ-NH1	-13.16	113.72	120.30
1	D	46	ARG	NE-CZ-NH2	13.03	126.82	120.30
1	D	46	ARG	NE-CZ-NH1	-12.57	114.02	120.30
1	A	183	ARG	NE-CZ-NH1	-12.47	114.07	120.30
1	A	183	ARG	NE-CZ-NH2	11.09	125.85	120.30
1	A	273	ARG	NE-CZ-NH1	10.70	125.65	120.30
1	B	273	ARG	NE-CZ-NH2	-10.69	114.95	120.30
1	B	273	ARG	NE-CZ-NH1	10.54	125.57	120.30
1	A	110	ARG	NE-CZ-NH2	10.19	125.40	120.30
1	B	134	TYR	CD1-CE1-CZ	9.95	128.75	119.80
1	A	273	ARG	NE-CZ-NH2	-9.73	115.43	120.30
1	C	288	TYR	CZ-CE2-CD2	9.10	127.99	119.80
1	D	365	TYR	CD1-CE1-CZ	8.87	127.78	119.80
1	D	365	TYR	CZ-CE2-CD2	8.79	127.71	119.80
1	B	134	TYR	CZ-CE2-CD2	8.78	127.71	119.80
1	C	288	TYR	CD1-CE1-CZ	8.75	127.68	119.80
1	A	110	ARG	NE-CZ-NH1	-8.41	116.10	120.30
1	B	134	TYR	CD1-CG-CD2	-8.32	108.75	117.90
1	B	134	TYR	CB-CG-CD2	8.15	125.89	121.00
1	B	134	TYR	CE1-CZ-CE2	-7.94	107.10	119.80
1	C	288	TYR	CD1-CG-CD2	-7.84	109.28	117.90
1	C	288	TYR	CE1-CZ-CE2	-7.82	107.30	119.80
1	C	62	TYR	CD1-CE1-CZ	7.68	126.72	119.80
1	D	365	TYR	CE1-CZ-CE2	-7.56	107.70	119.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	6	ARG	CD-NE-CZ	7.52	134.12	123.60
1	D	365	TYR	CD1-CG-CD2	-7.48	109.67	117.90
1	B	46	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	C	288	TYR	CB-CG-CD2	7.47	125.48	121.00
1	C	273	ARG	NE-CZ-NH1	-7.36	116.62	120.30
1	B	134	TYR	CB-CG-CD1	7.16	125.30	121.00
1	D	273	ARG	NE-CZ-NH1	-7.12	116.74	120.30
1	C	110	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	D	365	TYR	CB-CG-CD2	7.07	125.24	121.00
1	C	288	TYR	CB-CG-CD1	7.05	125.23	121.00
1	C	446	ASP	CB-CG-OD1	6.97	124.57	118.30
1	C	62	TYR	CZ-CE2-CD2	6.89	126.00	119.80
1	C	273	ARG	NE-CZ-NH2	6.87	123.73	120.30
1	D	365	TYR	CB-CG-CD1	6.82	125.09	121.00
1	C	446	ASP	CB-CG-OD2	6.78	124.40	118.30
1	B	46	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	D	110	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	C	446	ASP	OD1-CG-OD2	-6.54	110.87	123.30
1	C	110	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	B	110	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	A	183	ARG	CD-NE-CZ	6.27	132.38	123.60
1	D	273	ARG	NE-CZ-NH2	6.23	123.41	120.30
1	D	246	TYR	CD1-CE1-CZ	6.16	125.34	119.80
1	C	46	ARG	CD-NE-CZ	6.12	132.17	123.60
1	A	110	ARG	CD-NE-CZ	6.12	132.16	123.60
1	B	110	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	A	246	TYR	CD1-CE1-CZ	6.08	125.27	119.80
1	C	216	PHE	CD1-CG-CD2	-6.04	110.45	118.30
1	C	62	TYR	CE1-CZ-CE2	-6.02	110.16	119.80
1	C	246	TYR	CD1-CE1-CZ	5.98	125.18	119.80
1	C	216	PHE	CB-CG-CD1	5.96	124.97	120.80
1	C	62	TYR	CD1-CG-CD2	-5.91	111.41	117.90
1	D	246	TYR	CB-CG-CD2	5.91	124.54	121.00
1	A	246	TYR	CB-CG-CD2	5.90	124.54	121.00
1	C	62	TYR	CB-CG-CD2	5.88	124.53	121.00
1	B	244	ASP	CB-CG-OD2	5.87	123.59	118.30
1	A	273	ARG	CD-NE-CZ	5.87	131.81	123.60
1	B	246	TYR	CD1-CE1-CZ	5.84	125.06	119.80
1	C	216	PHE	CE1-CZ-CE2	-5.80	109.56	120.00
1	D	46	ARG	CD-NE-CZ	5.79	131.71	123.60
1	A	246	TYR	CZ-CE2-CD2	5.78	125.00	119.80
1	B	246	TYR	CB-CG-CD2	5.73	124.44	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	273	ARG	CD-NE-CZ	5.70	131.58	123.60
1	B	246	TYR	CD1-CG-CD2	-5.67	111.66	117.90
1	D	246	TYR	CD1-CG-CD2	-5.65	111.68	117.90
1	A	246	TYR	CD1-CG-CD2	-5.64	111.70	117.90
1	A	46	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	D	6	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	46	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	D	246	TYR	CZ-CE2-CD2	5.52	124.77	119.80
1	C	246	TYR	CD1-CG-CD2	-5.49	111.87	117.90
1	C	246	TYR	CB-CG-CD2	5.46	124.27	121.00
1	B	246	TYR	CZ-CE2-CD2	5.45	124.71	119.80
1	C	216	PHE	CB-CG-CD2	5.39	124.57	120.80
1	C	246	TYR	CZ-CE2-CD2	5.28	124.55	119.80
1	B	200	PHE	CD1-CG-CD2	-5.27	111.45	118.30
1	B	244	ASP	OD1-CG-OD2	-5.16	113.49	123.30
1	B	200	PHE	CB-CG-CD1	5.15	124.40	120.80
1	B	244	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	246	TYR	CE1-CZ-CE2	-5.12	111.61	119.80
1	C	62	TYR	CB-CG-CD1	5.10	124.06	121.00
1	B	6	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	D	110	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	B	200	PHE	CE1-CZ-CE2	-5.00	111.00	120.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3915	0	3721	34	1
1	B	3923	0	3725	26	0
1	C	3928	0	3740	44	1
1	D	3932	0	3732	33	0
2	A	43	0	30	2	0
2	B	43	0	30	2	0
2	C	43	0	30	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	43	0	30	0	0
3	A	48	0	26	1	0
3	B	48	0	26	2	0
3	C	48	0	26	1	0
3	D	48	0	26	1	0
4	A	130	0	0	1	0
4	B	136	0	0	1	0
4	C	116	0	0	1	0
4	D	104	0	0	0	0
All	All	16548	0	15142	120	1

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 4.

All (120) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:GLU:O	1:B:110:ARG:NH2	2.15	0.79
1:D:106:GLU:O	1:D:110:ARG:NH2	2.15	0.79
1:C:106:GLU:O	1:C:110:ARG:NH2	2.16	0.78
1:A:425:ALA:O	1:A:429:HIS:HD2	1.71	0.74
1:A:153:ARG:HB3	1:C:381:ARG:HD3	1.71	0.71
1:B:153:ARG:HB3	1:D:381:ARG:HD3	1.72	0.71
1:C:118:THR:O	4:C:688:HOH:O	2.08	0.71
1:C:51:GLU:HB3	1:C:100[A]:ARG:HE	1.55	0.70
1:B:425:ALA:O	1:B:429:HIS:HD2	1.74	0.69
1:B:12:GLY:HA2	1:C:362:HIS:HD2	1.59	0.66
1:A:362:HIS:HD2	1:D:12:GLY:HA2	1.61	0.66
1:A:433:ASP:O	1:A:437:GLN:HG2	1.95	0.66
1:C:49:ILE:O	1:C:100[A]:ARG:NH2	2.29	0.65
1:A:381:ARG:HD3	1:C:153:ARG:HB3	1.80	0.64
1:B:381:ARG:HD3	1:D:153:ARG:HB3	1.80	0.63
1:C:69:HIS:HD2	1:C:70:ASP:H	1.46	0.62
2:B:500:HEM:HBB2	2:B:500:HEM:HMB2	1.82	0.61
2:A:500:HEM:HBB2	2:A:500:HEM:HMB2	1.83	0.60
1:C:69:HIS:CD2	1:C:70:ASP:N	2.73	0.57
1:C:428:PHE:HD2	1:C:429:HIS:HD2	1.51	0.57
1:C:117:TYR:HB3	1:C:359:ARG:HG3	1.88	0.55
1:A:40:LYS:HE3	1:D:365:TYR:HE2	1.70	0.55
1:D:428:PHE:HD2	1:D:429:HIS:HD2	1.55	0.55
1:A:40:LYS:HE3	1:D:365:TYR:CE2	2.42	0.55

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:HIS:ND1	1:C:292:GLU:O	2.38	0.55
1:A:183:ARG:HD3	3:A:501:NDP:C6A	2.38	0.54
1:C:69:HIS:CD2	1:C:70:ASP:H	2.24	0.54
1:B:425:ALA:O	1:B:429:HIS:CD2	2.60	0.54
1:A:235:ALA:HB2	1:B:235:ALA:HB2	1.91	0.53
1:A:362:HIS:C	1:A:362:HIS:HD1	2.12	0.53
1:A:425:ALA:O	1:A:429:HIS:CD2	2.59	0.53
1:C:362:HIS:HD1	1:C:362:HIS:C	2.12	0.53
1:C:428:PHE:HD2	1:C:429:HIS:CD2	2.27	0.52
1:C:377:ASN:HB3	1:C:380:GLN:HB3	1.92	0.52
1:D:428:PHE:HD2	1:D:429:HIS:CD2	2.28	0.51
1:D:246:TYR:CE1	1:D:250:GLU:HG3	2.46	0.51
1:B:377:ASN:HB3	1:B:380:GLN:HB3	1.93	0.51
1:A:390:ASN:ND2	1:D:4:LYS:HB2	2.27	0.50
1:B:4:LYS:HB2	1:C:390:ASN:ND2	2.27	0.50
1:D:189:TYR:CE2	1:D:241:SER:HB3	2.47	0.50
1:B:100:ARG:HD3	4:B:730:HOH:O	2.11	0.49
1:A:448:ARG:NH2	1:A:477:LEU:HA	2.27	0.49
1:D:114:MET:HE3	1:D:125:LEU:HD23	1.93	0.49
1:B:54:OMT:HE3	1:B:145:ASN:HB2	1.94	0.49
1:A:377:ASN:HB3	1:A:380:GLN:HB3	1.95	0.49
1:A:4:LYS:HB2	1:D:390:ASN:ND2	2.28	0.48
1:C:428:PHE:CD2	1:C:429:HIS:HD2	2.31	0.48
1:A:373:VAL:HG21	1:D:373:VAL:HG21	1.96	0.48
1:D:377:ASN:HB3	1:D:380:GLN:HB3	1.95	0.48
1:B:12:GLY:HA2	1:C:362:HIS:CD2	2.46	0.47
1:C:114:MET:HE3	1:C:125:LEU:HB3	1.96	0.47
1:A:189:TYR:CE2	1:A:241:SER:HB3	2.50	0.47
1:A:246:TYR:CE1	1:A:250:GLU:HG3	2.49	0.47
1:C:62:TYR:CD2	1:C:300:ARG:NH2	2.83	0.47
1:A:107:ARG:HB2	1:A:185:LEU:HD22	1.96	0.47
1:B:390:ASN:ND2	1:C:4:LYS:HB2	2.30	0.47
1:D:183:ARG:HD2	3:D:501:NDP:C6A	2.45	0.46
1:C:62:TYR:HD2	1:C:300:ARG:NH2	2.12	0.46
1:A:362:HIS:CD2	1:D:12:GLY:HA2	2.46	0.46
1:B:147:VAL:HB	1:B:162:LYS:HA	1.98	0.46
3:C:501:NDP:N3A	3:C:501:NDP:H6N	2.30	0.46
1:A:147:VAL:HB	1:A:162:LYS:HA	1.97	0.46
1:C:362:HIS:C	1:C:362:HIS:ND1	2.70	0.46
1:C:153:ARG:HD3	1:D:246:TYR:OH	2.16	0.46
1:D:428:PHE:CD2	1:D:429:HIS:HD2	2.32	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:TYR:CE1	1:C:90:PHE:CD1	3.05	0.45
1:C:147:VAL:HB	1:C:162:LYS:HA	1.98	0.45
1:B:189:TYR:CE2	1:B:241:SER:HB3	2.52	0.45
1:C:117:TYR:HB3	1:C:359:ARG:CG	2.47	0.45
2:B:500:HEM:HBB2	2:B:500:HEM:CMB	2.46	0.45
1:B:183:ARG:HD2	3:B:501:NDP:C6A	2.46	0.45
1:D:117:TYR:HB3	1:D:359:ARG:HG2	1.98	0.44
1:D:147:VAL:HB	1:D:162:LYS:HA	1.98	0.44
1:A:114:MET:HE3	1:A:125:LEU:HD23	1.99	0.44
1:D:311:GLN:HB3	1:D:353:ILE:HD13	1.98	0.44
1:C:179:ASP:O	1:C:184:GLY:HA3	2.17	0.44
1:B:114:MET:HE3	1:B:125:LEU:HD23	1.99	0.44
1:B:373:VAL:HG21	1:C:373:VAL:HG21	2.00	0.44
1:A:54:OMT:HE1	1:A:54:OMT:HB3	1.84	0.44
1:C:246:TYR:OH	1:D:153:ARG:HD3	2.17	0.44
1:A:179:ASP:O	1:A:184:GLY:HA3	2.18	0.44
1:A:198:HIS:HB2	1:A:200:PHE:CE1	2.53	0.43
2:C:500:HEM:HMB2	2:C:500:HEM:HBB2	2.00	0.43
1:C:96:VAL:HG21	1:C:109:ILE:HB	2.00	0.43
1:D:107:ARG:HB2	1:D:185:LEU:HD22	2.00	0.43
1:B:427:LEU:HB2	3:B:501:NDP:O2D	2.17	0.43
1:C:189:TYR:CE2	1:C:241:SER:HB3	2.54	0.43
2:C:500:HEM:CMC	2:C:500:HEM:HBC2	2.49	0.43
1:A:362:HIS:C	1:A:362:HIS:ND1	2.71	0.43
1:A:54:OMT:HE3	1:A:145:ASN:HB2	2.00	0.43
1:B:96:VAL:HG21	1:B:109:ILE:HB	2.00	0.43
1:C:380:GLN:NE2	1:C:391:GLN:OE1	2.51	0.43
1:B:179:ASP:O	1:B:184:GLY:HA3	2.19	0.42
1:C:411:HIS:CE1	1:D:22:GLN:HG3	2.53	0.42
1:A:380:GLN:NE2	1:A:391:GLN:OE1	2.52	0.42
1:D:96:VAL:HG21	1:D:109:ILE:HB	2.01	0.42
1:A:311:GLN:HB3	1:A:353:ILE:HD13	2.02	0.42
1:B:395:GLN:NE2	1:C:6:ARG:HB3	2.34	0.42
1:B:243:ARG:O	1:B:247:GLU:HB2	2.20	0.42
1:B:125:LEU:HD12	1:B:125:LEU:HA	1.87	0.42
1:A:96:VAL:HG21	1:A:109:ILE:HB	2.01	0.42
1:B:339:GLY:O	1:B:343:ARG:HG3	2.19	0.42
1:C:24:ALA:O	1:C:28:GLY:HA3	2.20	0.42
1:C:246:TYR:CZ	1:D:154:THR:HG22	2.55	0.41
1:A:183:ARG:HD2	4:A:718:HOH:O	2.20	0.41
1:B:311:GLN:HB3	1:B:353:ILE:HD13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:OMT:HE3	1:C:145:ASN:HB2	2.01	0.41
2:C:500:HEM:HBC2	2:C:500:HEM:HMC2	2.03	0.41
1:D:198:HIS:HB2	1:D:200:PHE:CE1	2.56	0.41
1:D:431:PHE:O	1:D:436:LYS:NZ	2.53	0.41
1:C:46:ARG:HG2	1:D:344:TYR:CG	2.55	0.41
1:C:198:HIS:HB2	1:C:200:PHE:CE1	2.56	0.41
1:C:344:TYR:CG	1:D:46:ARG:HG2	2.56	0.41
1:D:243:ARG:O	1:D:247:GLU:HB2	2.21	0.41
1:C:62:TYR:CD1	1:C:90:PHE:HD1	2.38	0.40
1:A:444:ALA:O	1:A:448:ARG:HB2	2.21	0.40
1:A:453:GLN:OE1	1:A:457:ARG:NH2	2.54	0.40
1:D:24:ALA:O	1:D:28:GLY:HA3	2.21	0.40
1:A:92:ARG:HD3	2:A:500:HEM:O1D	2.20	0.40
1:C:107:ARG:HB2	1:C:185:LEU:HD22	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ASP:OD2	1:C:471:LYS:NZ[2_645]	1.95	0.25

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	476/484 (98%)	461 (97%)	15 (3%)	0	100	100
1	B	477/484 (99%)	463 (97%)	14 (3%)	0	100	100
1	C	478/484 (99%)	465 (97%)	13 (3%)	0	100	100
1	D	478/484 (99%)	465 (97%)	13 (3%)	0	100	100
All	All	1909/1936 (99%)	1854 (97%)	55 (3%)	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	409/412 (99%)	400 (98%)	9 (2%)	52	75
1	B	410/412 (100%)	404 (98%)	6 (2%)	65	83
1	C	411/412 (100%)	407 (99%)	4 (1%)	76	89
1	D	411/412 (100%)	405 (98%)	6 (2%)	65	83
All	All	1641/1648 (100%)	1616 (98%)	25 (2%)	65	83

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	GLU
1	A	185	LEU
1	A	251	LYS
1	A	273	ARG
1	A	360	CYS
1	A	362	HIS
1	A	448	ARG
1	A	453	GLN
1	A	469	TYR
1	B	119	GLU
1	B	185	LEU
1	B	273	ARG
1	B	359	ARG
1	B	453	GLN
1	B	469	TYR
1	C	119	GLU
1	C	185	LEU
1	C	362	HIS
1	C	469	TYR
1	D	119	GLU
1	D	185	LEU
1	D	202	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	247	GLU
1	D	457	ARG
1	D	469	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	429	HIS
1	B	429	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
1	OMT	A	54	1	8,9,10	0.89	1 (12%)	6,12,14	0.15	0
1	OMT	C	54	1	8,9,10	1.91	1 (12%)	6,12,14	0.14	0
1	OMT	B	54	1	8,9,10	1.01	1 (12%)	6,12,14	0.13	0
1	OMT	D	54	1	8,9,10	0.97	1 (12%)	6,12,14	0.18	0

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	54	1	-	4/7/8/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMT	C	54	1	-	4/7/8/10	-
1	OMT	B	54	1	-	3/7/8/10	-
1	OMT	D	54	1	-	3/7/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	54	OMT	CB-CA	5.28	1.60	1.53
1	B	54	OMT	CB-CA	2.75	1.57	1.53
1	D	54	OMT	CB-CA	2.53	1.56	1.53
1	A	54	OMT	CB-CA	2.32	1.56	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	54	OMT	O-C-CA-CB
1	A	54	OMT	CB-CG-SD-CE
1	A	54	OMT	CB-CG-SD-OD1
1	A	54	OMT	CB-CG-SD-OD2
1	B	54	OMT	O-C-CA-CB
1	B	54	OMT	CB-CG-SD-OD1
1	C	54	OMT	CB-CG-SD-CE
1	C	54	OMT	CB-CG-SD-OD1
1	C	54	OMT	CB-CG-SD-OD2
1	D	54	OMT	O-C-CA-CB
1	D	54	OMT	CB-CG-SD-OD1
1	B	54	OMT	CB-CG-SD-CE
1	D	54	OMT	CB-CG-SD-CE
1	C	54	OMT	N-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	54	OMT	2	0
1	C	54	OMT	1	0
1	B	54	OMT	1	0

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

8 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	B	500	1	41,50,50	1.89	8 (19%)	45,82,82	2.28	14 (31%)
3	NDP	A	501	-	45,52,52	0.65	2 (4%)	53,80,80	0.95	1 (1%)
2	HEM	A	500	1	41,50,50	1.94	6 (14%)	45,82,82	2.09	11 (24%)
3	NDP	B	501	-	45,52,52	0.62	1 (2%)	53,80,80	1.02	3 (5%)
2	HEM	C	500	1	41,50,50	1.92	8 (19%)	45,82,82	2.28	17 (37%)
3	NDP	C	501	-	45,52,52	0.73	2 (4%)	53,80,80	1.02	3 (5%)
3	NDP	D	501	-	45,52,52	0.63	0	53,80,80	0.95	1 (1%)
2	HEM	D	500	1	41,50,50	1.91	7 (17%)	45,82,82	2.17	10 (22%)

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	B	500	1	-	3/12/54/54	-
3	NDP	A	501	-	-	9/30/77/77	0/5/5/5
2	HEM	A	500	1	-	4/12/54/54	-
3	NDP	B	501	-	-	8/30/77/77	0/5/5/5
2	HEM	C	500	1	-	4/12/54/54	-
3	NDP	C	501	-	-	9/30/77/77	0/5/5/5
3	NDP	D	501	-	-	10/30/77/77	0/5/5/5
2	HEM	D	500	1	-	2/12/54/54	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C3D-C2D	8.24	1.54	1.36
2	C	500	HEM	C3D-C2D	8.13	1.54	1.36
2	D	500	HEM	C3D-C2D	8.06	1.53	1.36
2	B	500	HEM	C3D-C2D	7.98	1.53	1.36
2	A	500	HEM	C3C-C2C	-3.81	1.35	1.40
2	A	500	HEM	C3C-CAC	3.73	1.55	1.47
2	D	500	HEM	C3C-C2C	-3.64	1.35	1.40
2	C	500	HEM	C3C-C2C	-3.62	1.35	1.40
2	B	500	HEM	C3C-CAC	3.55	1.55	1.47
2	D	500	HEM	C3C-CAC	3.54	1.55	1.47
2	B	500	HEM	C3C-C2C	-3.48	1.35	1.40
2	C	500	HEM	C3C-CAC	3.26	1.54	1.47
2	C	500	HEM	FE-NB	3.20	2.12	1.96
2	A	500	HEM	CAB-C3B	3.05	1.55	1.47
3	C	501	NDP	C7N-C3N	2.84	1.54	1.48
2	D	500	HEM	CAB-C3B	2.74	1.54	1.47
2	C	500	HEM	CAB-C3B	2.64	1.54	1.47
2	A	500	HEM	FE-NB	2.60	2.09	1.96
2	B	500	HEM	CAB-C3B	2.57	1.54	1.47
2	B	500	HEM	FE-ND	2.50	2.09	1.96
3	A	501	NDP	C6N-N1N	2.48	1.43	1.37
2	D	500	HEM	FE-ND	2.47	2.09	1.96
2	C	500	HEM	FE-ND	2.33	2.08	1.96
3	C	501	NDP	C6N-N1N	2.32	1.43	1.37
2	B	500	HEM	CMB-C2B	2.29	1.55	1.50
2	C	500	HEM	CHA-C4D	2.22	1.40	1.35
2	D	500	HEM	CAA-C2A	2.14	1.55	1.52
2	B	500	HEM	FE-NB	2.13	2.07	1.96
2	D	500	HEM	CMB-C2B	2.09	1.55	1.50
2	A	500	HEM	CMD-C2D	2.09	1.55	1.50
2	C	500	HEM	CMB-C2B	2.07	1.55	1.50
3	B	501	NDP	C6N-N1N	2.05	1.42	1.37
3	A	501	NDP	C8A-N7A	-2.04	1.31	1.34
2	B	500	HEM	CMA-C3A	2.01	1.55	1.51

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	HEM	C4D-ND-C1D	7.58	112.91	105.07
2	B	500	HEM	C4D-ND-C1D	7.30	112.61	105.07
2	A	500	HEM	C4D-ND-C1D	7.13	112.44	105.07
2	D	500	HEM	C4D-ND-C1D	6.70	112.00	105.07

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	HEM	CBA-CAA-C2A	-5.61	103.05	112.62
2	B	500	HEM	CAD-CBD-CGD	-5.49	101.80	113.60
2	D	500	HEM	CBA-CAA-C2A	-5.38	103.43	112.62
2	A	500	HEM	CBA-CAA-C2A	-5.18	103.77	112.62
2	B	500	HEM	CBA-CAA-C2A	-4.77	104.48	112.62
2	D	500	HEM	C4C-CHD-C1D	4.60	128.63	122.56
2	A	500	HEM	CAD-CBD-CGD	-4.52	103.87	113.60
2	D	500	HEM	CAD-CBD-CGD	-4.48	103.95	113.60
2	C	500	HEM	C4C-CHD-C1D	4.34	128.29	122.56
2	B	500	HEM	C4C-CHD-C1D	4.29	128.22	122.56
2	C	500	HEM	C1B-NB-C4B	4.00	109.21	105.07
2	C	500	HEM	CAD-CBD-CGD	-3.99	105.02	113.60
2	B	500	HEM	C1B-NB-C4B	3.46	108.65	105.07
2	D	500	HEM	C1B-NB-C4B	3.40	108.58	105.07
2	A	500	HEM	C1B-NB-C4B	3.31	108.50	105.07
2	A	500	HEM	C4C-CHD-C1D	3.28	126.89	122.56
3	B	501	NDP	C4A-C5A-N7A	3.02	112.55	109.40
2	C	500	HEM	C2C-C3C-C4C	2.90	108.92	106.90
2	B	500	HEM	C4B-CHC-C1C	2.88	126.36	122.56
2	B	500	HEM	CMA-C3A-C4A	-2.85	124.09	128.46
2	B	500	HEM	CHD-C1D-ND	2.83	127.51	124.43
3	D	501	NDP	C4A-C5A-N7A	2.80	112.31	109.40
2	B	500	HEM	C3D-C4D-ND	-2.68	107.19	110.17
2	C	500	HEM	CHC-C4B-NB	2.60	127.25	124.43
2	C	500	HEM	C3D-C4D-ND	-2.57	107.30	110.17
2	C	500	HEM	C4B-CHC-C1C	2.57	125.95	122.56
2	D	500	HEM	CMC-C2C-C3C	2.57	129.49	124.68
2	D	500	HEM	CHC-C4B-NB	2.53	127.19	124.43
2	B	500	HEM	CMC-C2C-C3C	2.50	129.36	124.68
2	A	500	HEM	CHA-C4D-ND	2.48	127.45	124.38
3	A	501	NDP	O7N-C7N-C3N	-2.47	116.24	120.90
2	A	500	HEM	CMC-C2C-C3C	2.46	129.29	124.68
3	C	501	NDP	O2A-PA-O1A	2.46	124.40	112.24
2	B	500	HEM	CBD-CAD-C3D	-2.44	105.85	112.63
3	C	501	NDP	C5A-C6A-N6A	2.43	124.05	120.35
2	D	500	HEM	C2C-C3C-C4C	2.42	108.59	106.90
2	A	500	HEM	C1D-C2D-C3D	-2.42	104.42	106.96
2	D	500	HEM	C4A-C3A-C2A	2.33	108.61	107.00
3	B	501	NDP	C5A-C6A-N6A	2.31	123.86	120.35
2	A	500	HEM	C3D-C4D-ND	-2.30	107.60	110.17
2	A	500	HEM	C4B-CHC-C1C	2.30	125.59	122.56
2	B	500	HEM	O1D-CGD-CBD	-2.29	115.73	123.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	HEM	CMA-C3A-C4A	-2.28	124.96	128.46
2	C	500	HEM	O1A-CGA-CBA	-2.25	115.86	123.08
2	A	500	HEM	O1D-CGD-CBD	-2.21	115.99	123.08
2	C	500	HEM	C4B-C3B-C2B	2.19	108.85	107.11
2	C	500	HEM	CMC-C2C-C3C	2.18	128.76	124.68
2	C	500	HEM	CHD-C1D-ND	2.17	126.79	124.43
2	C	500	HEM	C2B-C1B-NB	-2.16	107.28	109.84
2	B	500	HEM	C2C-C3C-C4C	2.13	108.39	106.90
2	B	500	HEM	C4B-C3B-C2B	2.12	108.80	107.11
2	C	500	HEM	O2A-CGA-CBA	2.12	120.83	114.03
2	C	500	HEM	C3C-C4C-NC	-2.10	106.98	110.94
2	C	500	HEM	CBD-CAD-C3D	-2.08	106.86	112.63
3	B	501	NDP	C1D-N1N-C2N	-2.04	117.72	121.11
3	C	501	NDP	O2N-PN-O1N	2.01	122.17	112.24

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	NDP	PN-O3-PA-O5B
3	A	501	NDP	C5D-O5D-PN-O3
3	B	501	NDP	PN-O3-PA-O5B
3	B	501	NDP	PA-O3-PN-O5D
3	C	501	NDP	C5B-O5B-PA-O3
3	C	501	NDP	C2B-O2B-P2B-O3X
3	C	501	NDP	C5D-O5D-PN-O3
3	C	501	NDP	C5D-O5D-PN-O1N
3	D	501	NDP	C5D-O5D-PN-O3
3	A	501	NDP	C3B-C2B-O2B-P2B
3	A	501	NDP	C1B-C2B-O2B-P2B
3	B	501	NDP	C3B-C2B-O2B-P2B
3	A	501	NDP	O4D-C1D-N1N-C6N
3	C	501	NDP	O4D-C1D-N1N-C6N
3	D	501	NDP	PN-O3-PA-O5B
3	B	501	NDP	C1B-C2B-O2B-P2B
3	D	501	NDP	C2B-O2B-P2B-O3X
3	B	501	NDP	O4D-C1D-N1N-C6N
3	A	501	NDP	C5D-O5D-PN-O1N
3	A	501	NDP	C5D-O5D-PN-O2N
3	C	501	NDP	C5B-O5B-PA-O1A
3	C	501	NDP	C5B-O5B-PA-O2A
3	C	501	NDP	C5D-O5D-PN-O2N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	501	NDP	C5D-O5D-PN-O1N
3	D	501	NDP	C5D-O5D-PN-O2N
3	D	501	NDP	O4B-C4B-C5B-O5B
3	D	501	NDP	O4D-C1D-N1N-C6N
2	C	500	HEM	CAA-CBA-CGA-O1A
3	D	501	NDP	C3B-C2B-O2B-P2B
2	B	500	HEM	CAD-CBD-CGD-O2D
2	A	500	HEM	CAD-CBD-CGD-O1D
3	D	501	NDP	C1B-C2B-O2B-P2B
2	C	500	HEM	CAA-CBA-CGA-O2A
2	B	500	HEM	CAD-CBD-CGD-O1D
2	A	500	HEM	CAD-CBD-CGD-O2D
2	D	500	HEM	CAD-CBD-CGD-O2D
2	C	500	HEM	CAD-CBD-CGD-O2D
2	D	500	HEM	CAD-CBD-CGD-O1D
2	A	500	HEM	CAA-CBA-CGA-O1A
2	C	500	HEM	CAD-CBD-CGD-O1D
3	A	501	NDP	C2B-O2B-P2B-O2X
3	B	501	NDP	C2B-O2B-P2B-O2X
3	C	501	NDP	O4B-C4B-C5B-O5B
3	B	501	NDP	PN-O3-PA-O1A
2	A	500	HEM	CAA-CBA-CGA-O2A
3	D	501	NDP	C2N-C3N-C7N-N7N
3	A	501	NDP	O4B-C4B-C5B-O5B
3	B	501	NDP	O4B-C4B-C5B-O5B
2	B	500	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	HEM	2	0
3	A	501	NDP	1	0
2	A	500	HEM	2	0
3	B	501	NDP	2	0
2	C	500	HEM	3	0
3	C	501	NDP	1	0
3	D	501	NDP	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 then 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.

Ligand HEM B 500

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 500

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP B 501

Bond lengths

Bond angles

Torsions

Rings

Full wwPDB X-ray Structure Validation Report

Ligand HEM C 500

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP C 501

Bond lengths

Bond angles

Torsions

Rings

Full wwPDB X-ray Structure Validation Report

Ligand NDP D 501

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM D 500

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	478/484 (98%)	-0.54	1 (0%)	95	96	20, 27, 37, 60	3 (0%)
1	B	479/484 (98%)	-0.52	2 (0%)	92	93	21, 29, 40, 64	5 (1%)
1	C	478/484 (98%)	-0.42	3 (0%)	89	90	22, 32, 44, 92	4 (0%)
1	D	479/484 (98%)	-0.45	1 (0%)	95	96	23, 30, 40, 66	2 (0%)
All	All	1914/1936 (98%)	-0.48	7 (0%)	92	93	20, 29, 42, 92	14 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	482	ASP	4.6
1	B	361	PRO	2.4
1	B	359	ARG	2.3
1	C	433	ASP	2.1
1	A	480	LYS	2.1
1	D	3	GLU	2.1
1	C	480	LYS	2.0

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	D	54	10/11	0.93	0.15	26,31,39,45	0
1	OMT	B	54	10/11	0.94	0.15	24,28,45,49	0
1	OMT	A	54	10/11	0.95	0.13	23,27,41,43	0
1	OMT	C	54	10/11	0.96	0.14	28,34,44,47	0

6.3 Carbohydrates ⓘ

There are no monosaccharides 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(Å^2)	Q<0.9
3	NDP	C	501	48/48	0.94	0.23	42,49,55,62	0
3	NDP	B	501	48/48	0.95	0.15	31,38,42,47	0
3	NDP	A	501	48/48	0.95	0.16	29,37,41,45	0
2	HEM	B	500	43/43	0.96	0.12	20,24,27,41	0
2	HEM	C	500	43/43	0.96	0.13	22,26,28,45	0
2	HEM	D	500	43/43	0.96	0.13	22,26,30,44	0
3	NDP	D	501	48/48	0.96	0.13	32,40,45,52	0
2	HEM	A	500	43/43	0.97	0.11	18,23,25,41	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.
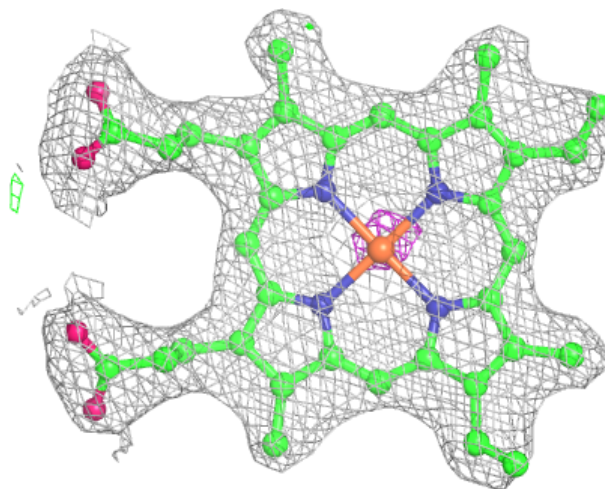
Electron density around NDP C 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
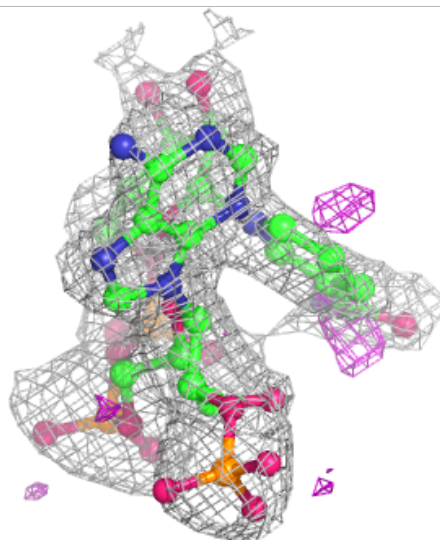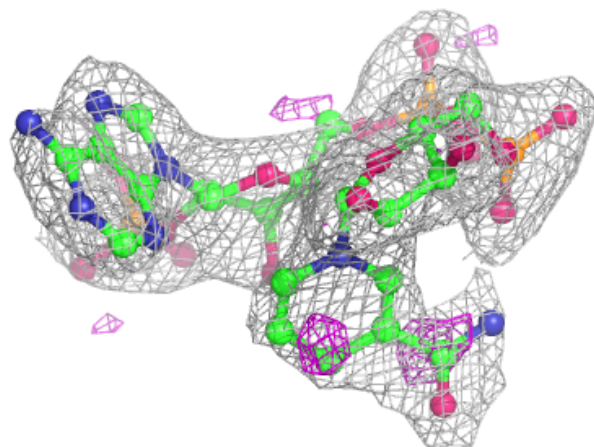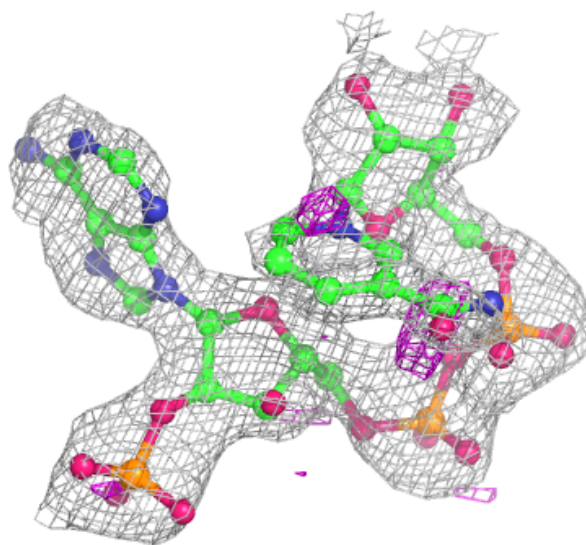
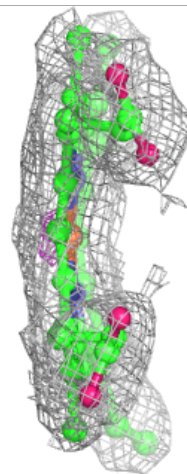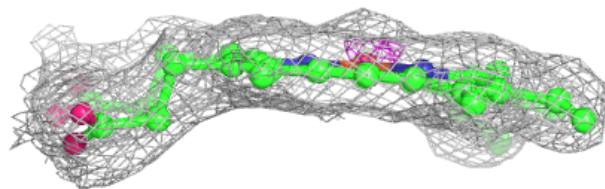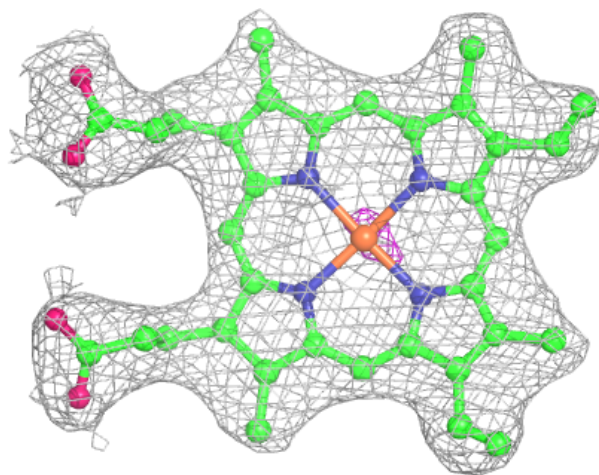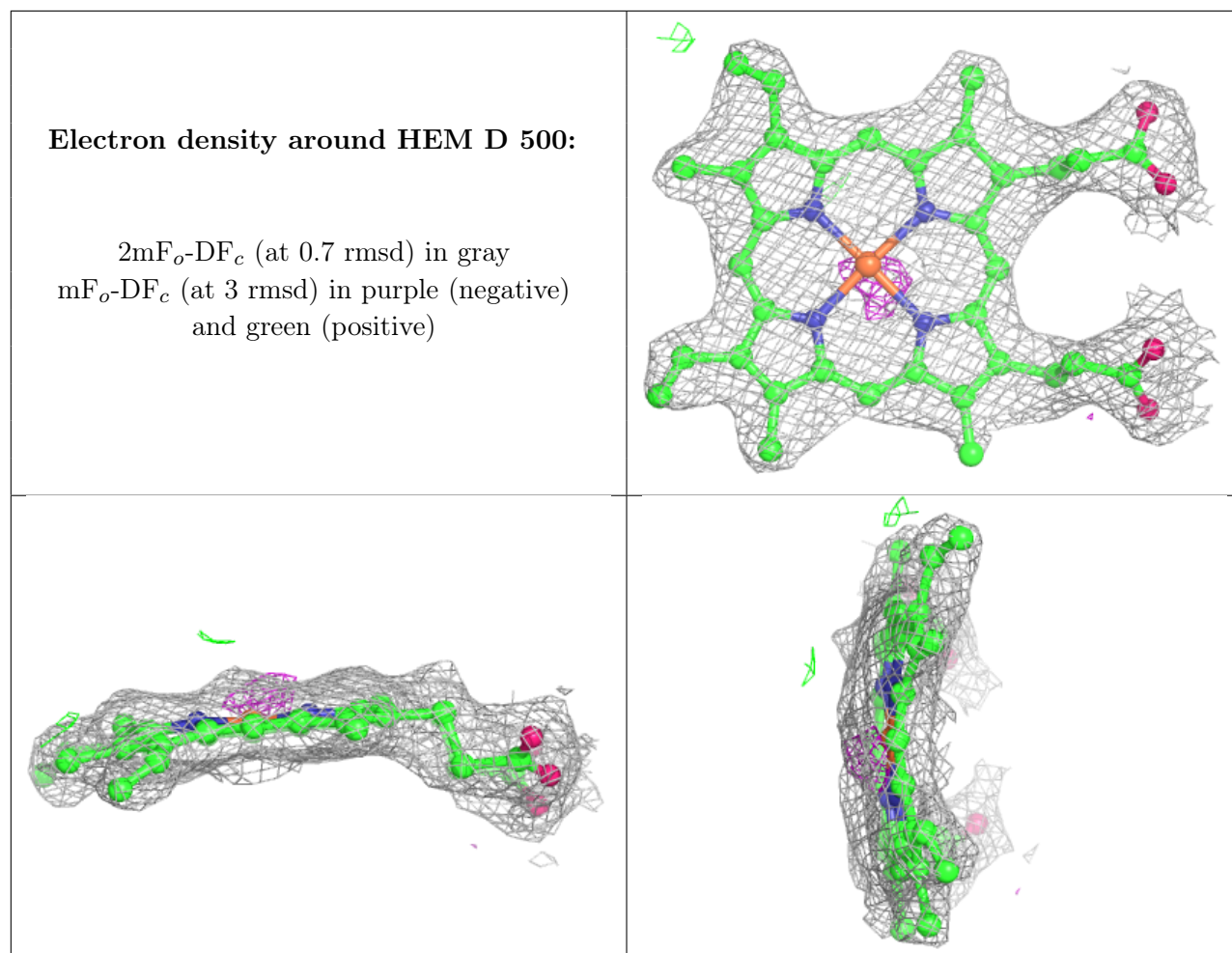**Electron density around NDP B 501:**

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
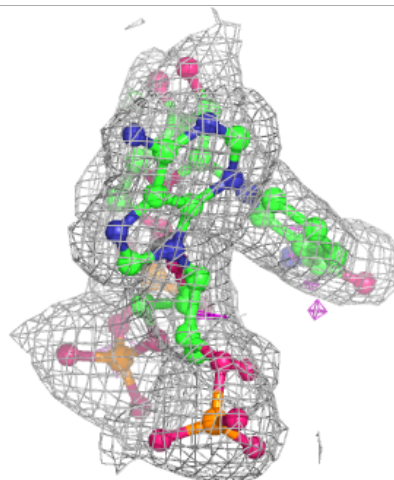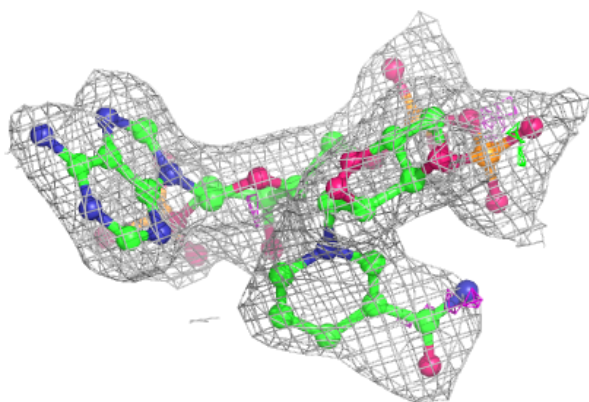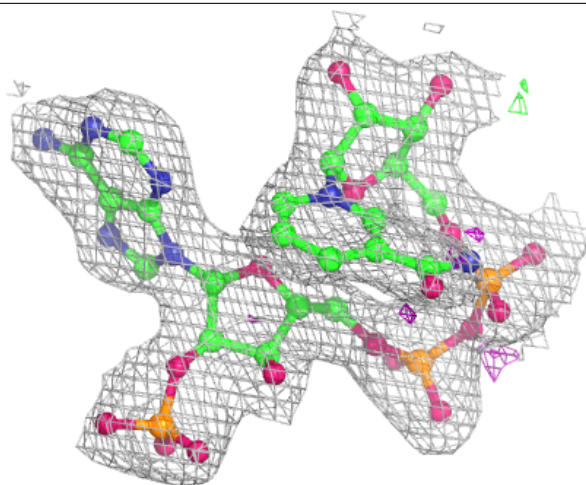
Electron density around NDP A 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
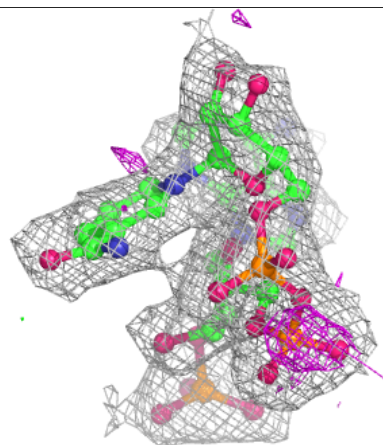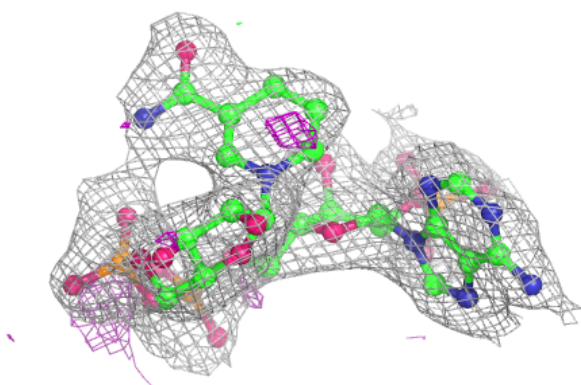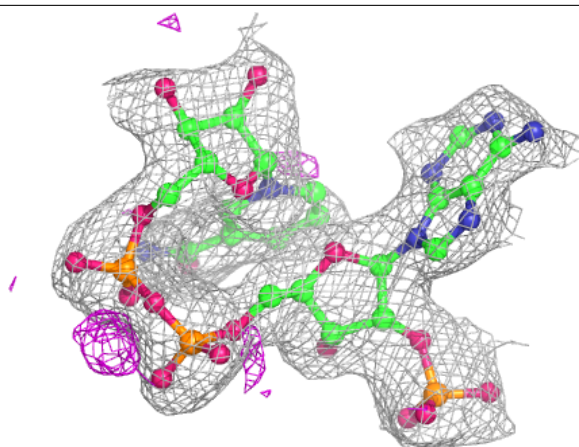
Electron density around HEM B 500:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
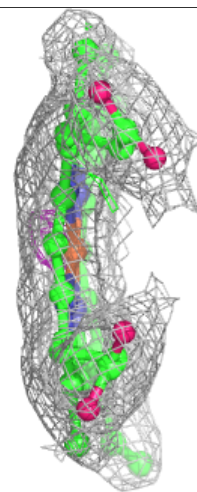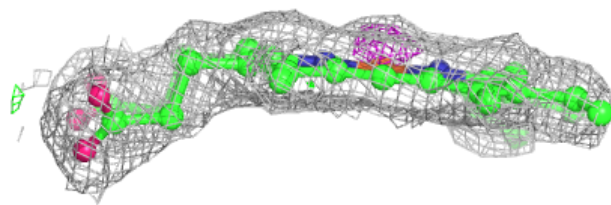
Electron density around HEM C 500:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around HEM D 500:

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

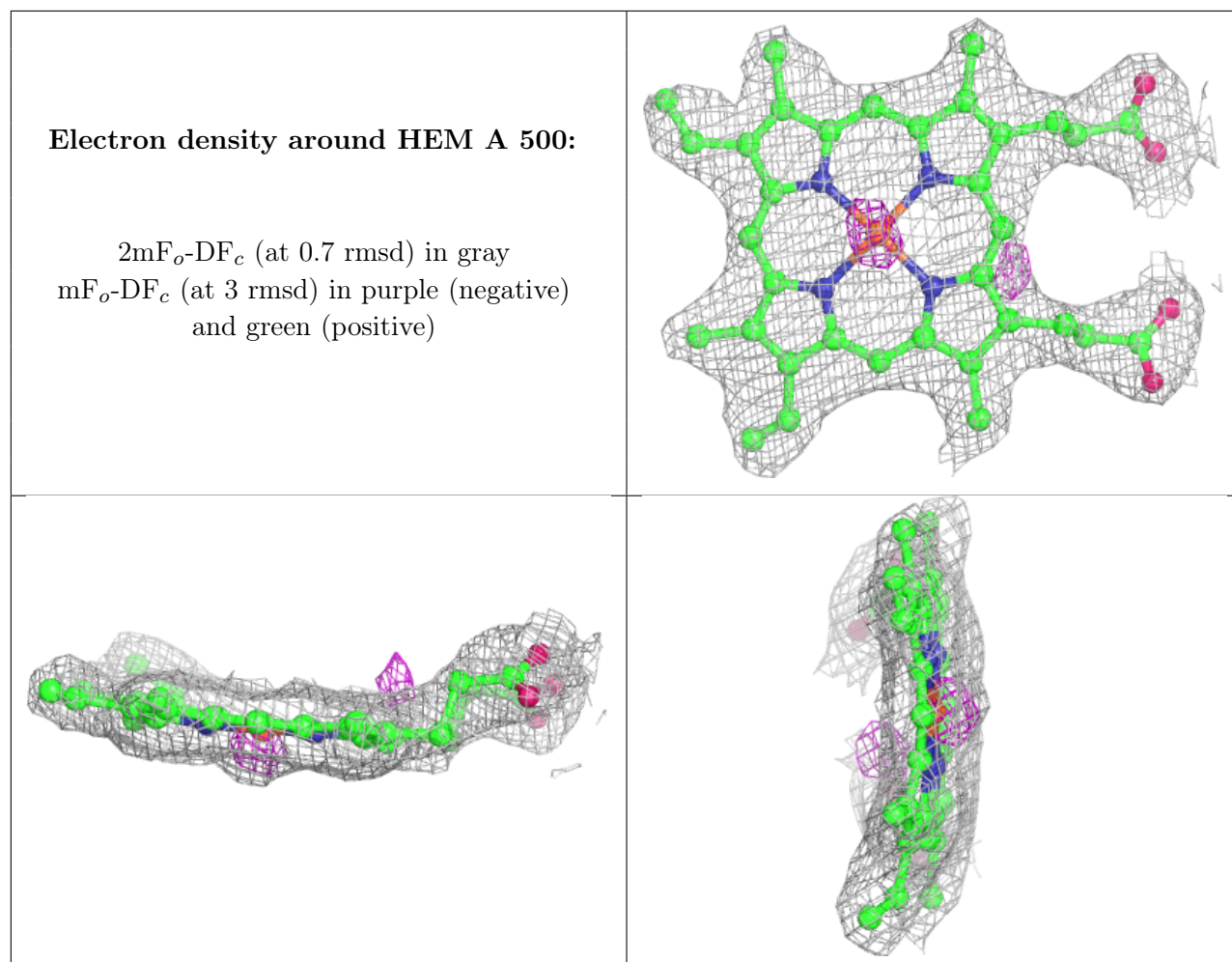**Electron density around NDP D 501:**

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

Electron density around HEM A 500:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
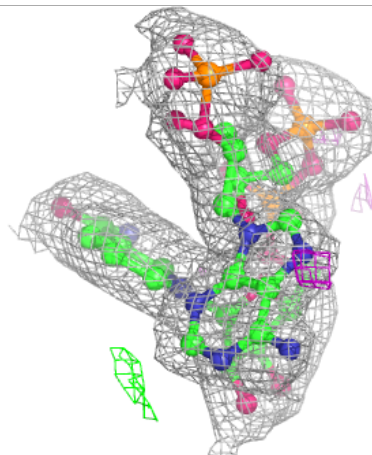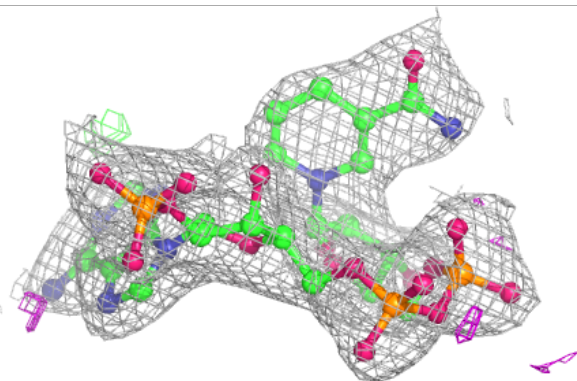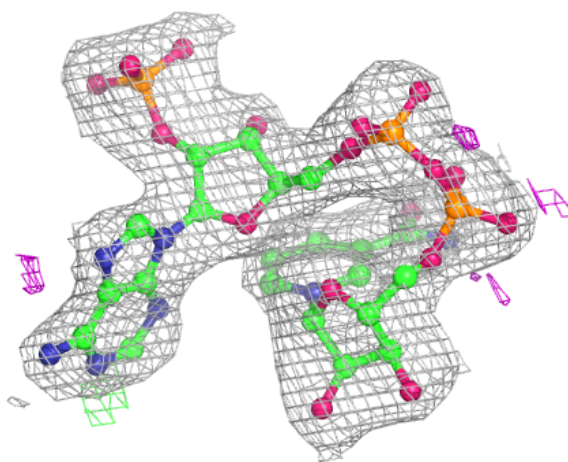
6.5   Other polymers (i)

There are no such residues in this entry.