Full wwPDB X-ray Structure Validation Report (i)

Jan 15, 2024 – 11:10 am GMT

|		
PDB ID	:	6RJR
Title	:	Crystal structure of a Fungal Catalase at 1.9 Angstrom
Authors	:	Gomez, S.; Navas-Yuste, S.; Payne, A.M.; Rivera, W.; Lopez-Estepa, M.; Brangbour, C.; Fulla, D.; Juanhuix, J.; Fernandez, F.J.; Vega, M.C.
Deposited on	:	2019-04-29
Resolution	:	1.90 Å(reported)

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
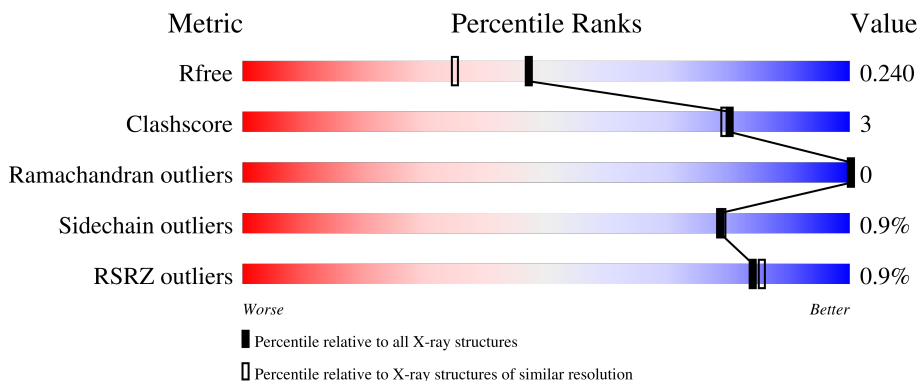
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	537	87% 7% 6%
1	B	537	88% 5% 7%
1	C	537	87% 6% 7%
1	D	537	87% 6% 7%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 17864 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	505	Total	C	N	O	S	0	3	0
			4060	2561	724	759	16			
1	B	501	Total	C	N	O	S	0	2	0
			4026	2539	717	753	17			
1	C	500	Total	C	N	O	S	0	5	0
			4039	2546	719	757	17			
1	D	502	Total	C	N	O	S	0	2	0
			4038	2546	722	754	16			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	initiating methionine	UNP Q6CR58
A	-24	LYS	-	expression tag	UNP Q6CR58
A	-23	HIS	-	expression tag	UNP Q6CR58
A	-22	HIS	-	expression tag	UNP Q6CR58
A	-21	HIS	-	expression tag	UNP Q6CR58
A	-20	HIS	-	expression tag	UNP Q6CR58
A	-19	HIS	-	expression tag	UNP Q6CR58
A	-18	HIS	-	expression tag	UNP Q6CR58
A	-17	PRO	-	expression tag	UNP Q6CR58
A	-16	MET	-	expression tag	UNP Q6CR58
A	-15	SER	-	expression tag	UNP Q6CR58
A	-14	ASP	-	expression tag	UNP Q6CR58
A	-13	TYR	-	expression tag	UNP Q6CR58
A	-12	ASP	-	expression tag	UNP Q6CR58
A	-11	ILE	-	expression tag	UNP Q6CR58
A	-10	PRO	-	expression tag	UNP Q6CR58
A	-9	THR	-	expression tag	UNP Q6CR58
A	-8	THR	-	expression tag	UNP Q6CR58
A	-7	GLU	-	expression tag	UNP Q6CR58
A	-6	ASN	-	expression tag	UNP Q6CR58
A	-5	LEU	-	expression tag	UNP Q6CR58

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	TYR	-	expression tag	UNP Q6CR58
A	-3	PHE	-	expression tag	UNP Q6CR58
A	-2	GLN	-	expression tag	UNP Q6CR58
A	-1	GLY	-	expression tag	UNP Q6CR58
A	0	ALA	-	expression tag	UNP Q6CR58
B	-25	MET	-	initiating methionine	UNP Q6CR58
B	-24	LYS	-	expression tag	UNP Q6CR58
B	-23	HIS	-	expression tag	UNP Q6CR58
B	-22	HIS	-	expression tag	UNP Q6CR58
B	-21	HIS	-	expression tag	UNP Q6CR58
B	-20	HIS	-	expression tag	UNP Q6CR58
B	-19	HIS	-	expression tag	UNP Q6CR58
B	-18	HIS	-	expression tag	UNP Q6CR58
B	-17	PRO	-	expression tag	UNP Q6CR58
B	-16	MET	-	expression tag	UNP Q6CR58
B	-15	SER	-	expression tag	UNP Q6CR58
B	-14	ASP	-	expression tag	UNP Q6CR58
B	-13	TYR	-	expression tag	UNP Q6CR58
B	-12	ASP	-	expression tag	UNP Q6CR58
B	-11	ILE	-	expression tag	UNP Q6CR58
B	-10	PRO	-	expression tag	UNP Q6CR58
B	-9	THR	-	expression tag	UNP Q6CR58
B	-8	THR	-	expression tag	UNP Q6CR58
B	-7	GLU	-	expression tag	UNP Q6CR58
B	-6	ASN	-	expression tag	UNP Q6CR58
B	-5	LEU	-	expression tag	UNP Q6CR58
B	-4	TYR	-	expression tag	UNP Q6CR58
B	-3	PHE	-	expression tag	UNP Q6CR58
B	-2	GLN	-	expression tag	UNP Q6CR58
B	-1	GLY	-	expression tag	UNP Q6CR58
B	0	ALA	-	expression tag	UNP Q6CR58
C	-25	MET	-	initiating methionine	UNP Q6CR58
C	-24	LYS	-	expression tag	UNP Q6CR58
C	-23	HIS	-	expression tag	UNP Q6CR58
C	-22	HIS	-	expression tag	UNP Q6CR58
C	-21	HIS	-	expression tag	UNP Q6CR58
C	-20	HIS	-	expression tag	UNP Q6CR58
C	-19	HIS	-	expression tag	UNP Q6CR58
C	-18	HIS	-	expression tag	UNP Q6CR58
C	-17	PRO	-	expression tag	UNP Q6CR58
C	-16	MET	-	expression tag	UNP Q6CR58
C	-15	SER	-	expression tag	UNP Q6CR58

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| Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	ASP	-	expression tag	UNP Q6CR58
C	-13	TYR	-	expression tag	UNP Q6CR58
C	-12	ASP	-	expression tag	UNP Q6CR58
C	-11	ILE	-	expression tag	UNP Q6CR58
C	-10	PRO	-	expression tag	UNP Q6CR58
C	-9	THR	-	expression tag	UNP Q6CR58
C	-8	THR	-	expression tag	UNP Q6CR58
C	-7	GLU	-	expression tag	UNP Q6CR58
C	-6	ASN	-	expression tag	UNP Q6CR58
C	-5	LEU	-	expression tag	UNP Q6CR58
C	-4	TYR	-	expression tag	UNP Q6CR58
C	-3	PHE	-	expression tag	UNP Q6CR58
C	-2	GLN	-	expression tag	UNP Q6CR58
C	-1	GLY	-	expression tag	UNP Q6CR58
C	0	ALA	-	expression tag	UNP Q6CR58
D	-25	MET	-	initiating methionine	UNP Q6CR58
D	-24	LYS	-	expression tag	UNP Q6CR58
D	-23	HIS	-	expression tag	UNP Q6CR58
D	-22	HIS	-	expression tag	UNP Q6CR58
D	-21	HIS	-	expression tag	UNP Q6CR58
D	-20	HIS	-	expression tag	UNP Q6CR58
D	-19	HIS	-	expression tag	UNP Q6CR58
D	-18	HIS	-	expression tag	UNP Q6CR58
D	-17	PRO	-	expression tag	UNP Q6CR58
D	-16	MET	-	expression tag	UNP Q6CR58
D	-15	SER	-	expression tag	UNP Q6CR58
D	-14	ASP	-	expression tag	UNP Q6CR58
D	-13	TYR	-	expression tag	UNP Q6CR58
D	-12	ASP	-	expression tag	UNP Q6CR58
D	-11	ILE	-	expression tag	UNP Q6CR58
D	-10	PRO	-	expression tag	UNP Q6CR58
D	-9	THR	-	expression tag	UNP Q6CR58
D	-8	THR	-	expression tag	UNP Q6CR58
D	-7	GLU	-	expression tag	UNP Q6CR58
D	-6	ASN	-	expression tag	UNP Q6CR58
D	-5	LEU	-	expression tag	UNP Q6CR58
D	-4	TYR	-	expression tag	UNP Q6CR58
D	-3	PHE	-	expression tag	UNP Q6CR58
D	-2	GLN	-	expression tag	UNP Q6CR58
D	-1	GLY	-	expression tag	UNP Q6CR58
D	0	ALA	-	expression tag	UNP Q6CR58

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

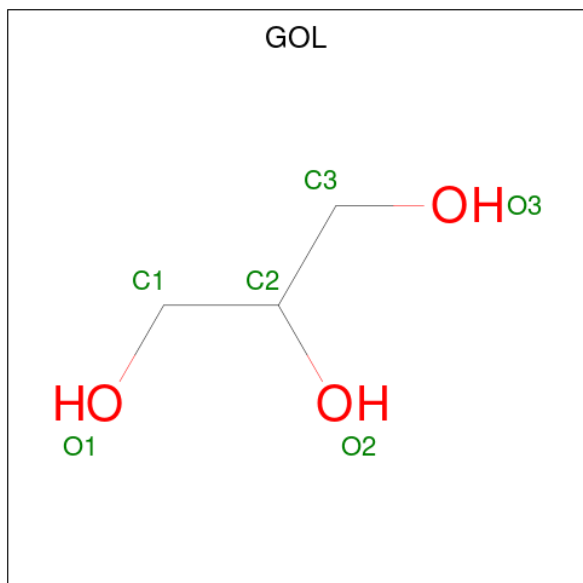mula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).
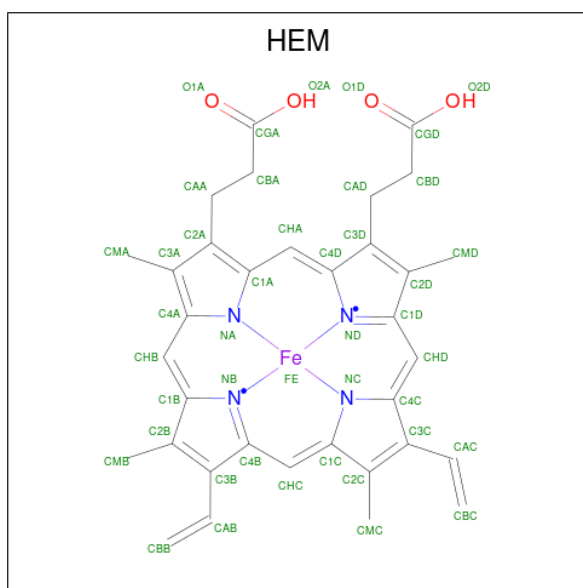
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).

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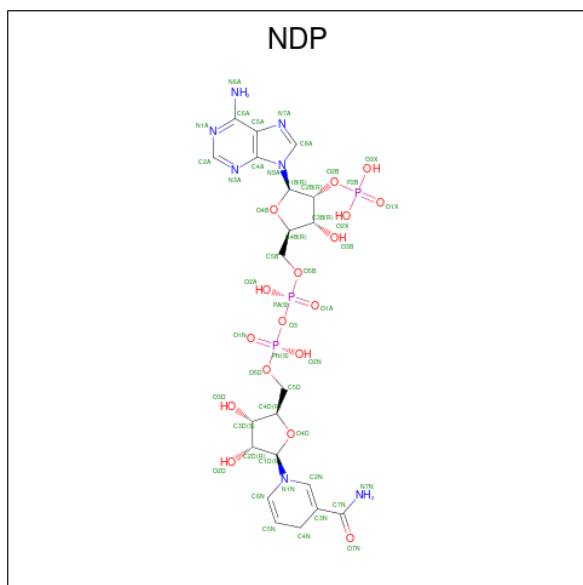
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	K 1	0	0
5	B	1	Total 1	K 1	0	0
5	C	1	Total 1	K 1	0	0
5	D	1	Total 1	K 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	Cl 1	0	0
6	D	1	Total 1	Cl 1	0	0

- Molecule 7 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	374	Total 378	O 378	0	4
7	B	253	Total 255	O 255	0	2
7	C	301	Total 305	O 305	0	4
7	D	325	Total 327	O 327	0	2

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.
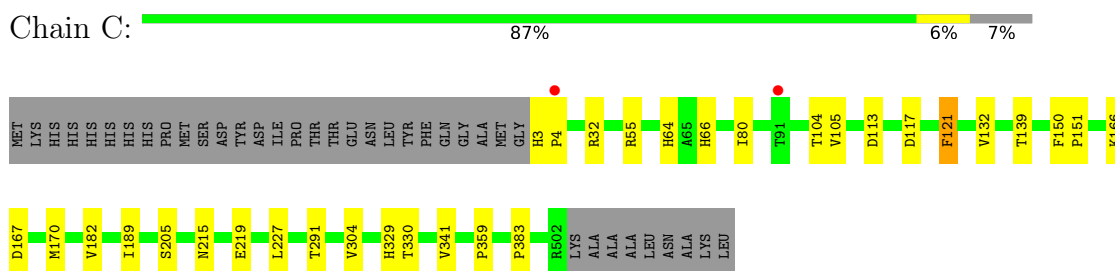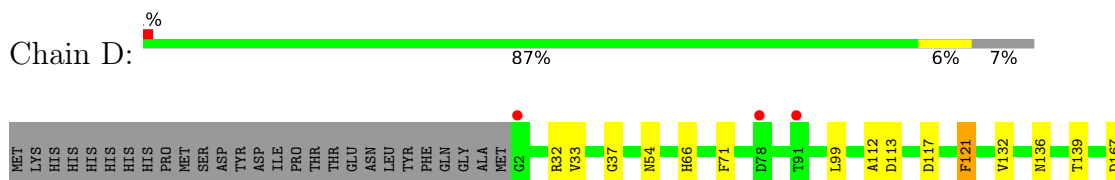
• Molecule 1: Catalase

Chain A:

• Molecule 1: Catalase

Chain B:

• Molecule 1: Catalase

Chain C:

• Molecule 1: Catalase

Chain D:
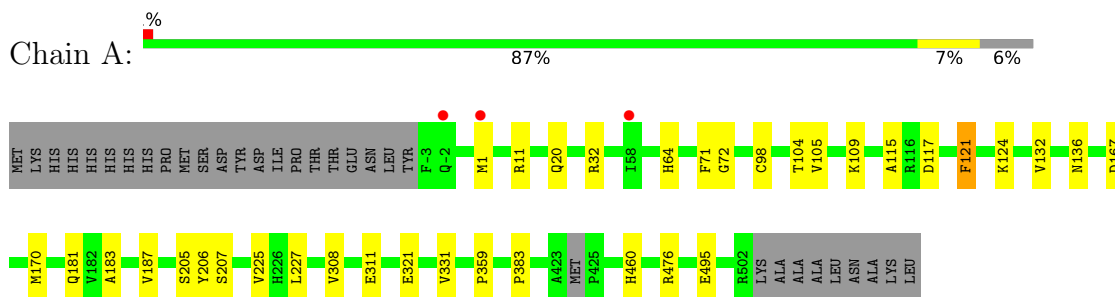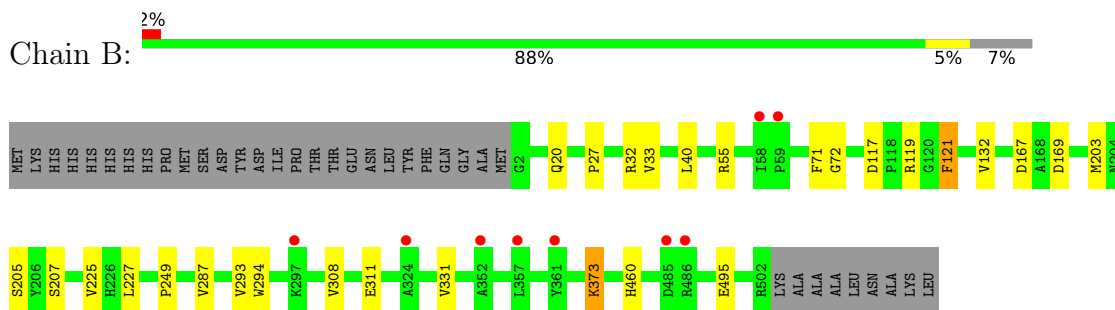
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	96.67Å 131.62Å 176.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.98 – 1.90 46.98 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.98-1.90) 98.9 (46.98-1.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.181 , 0.241 0.187 , 0.240	Depositor DCC
R_{free} test set	8833 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	21.4	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 55.9	EDS
L-test for twinning[2]	$< |L| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17864	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: K, HEM, CL, GOL, 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	0.62	0/4175	0.70	0/5667
1	B	0.56	0/4141	0.65	0/5625
1	C	0.60	0/4154	0.67	0/5645
1	D	0.61	0/4153	0.68	0/5640
All	All	0.60	0/16623	0.68	0/22577

There are no bond length outliers.

There are no bond angle outliers.

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	4060	0	3901	22	0
1	B	4026	0	3866	19	0
1	C	4039	0	3876	19	0
1	D	4038	0	3883	22	0
2	A	43	0	30	2	0
2	B	43	0	30	1	0
2	C	43	0	30	4	0
2	D	43	0	30	3	0
3	A	48	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	48	0	26	1	0
3	C	48	0	26	0	0
3	D	48	0	26	0	0
4	A	36	0	48	6	0
4	B	6	0	8	0	0
4	C	12	0	16	1	0
4	D	12	0	16	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	A	378	0	0	5	0
7	B	255	0	0	0	0
7	C	305	0	0	3	0
7	D	327	0	0	2	0
All	All	17864	0	15838	89	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 3.

All (89) 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)
2:C:601:HEM:HMB2	2:C:601:HEM:HBB2	1.64	0.80
2:A:601:HEM:HBB2	2:A:601:HEM:HMB2	1.72	0.70
2:D:602:HEM:HMB1	2:D:602:HEM:HBB2	1.74	0.68
2:C:601:HEM:HBB2	2:C:601:HEM:CMB	2.26	0.65
1:B:119:ARG:HB2	1:B:203:MET:HE1	1.81	0.63
2:A:601:HEM:HBB2	2:A:601:HEM:CMB	2.29	0.62
1:A:121:PHE:CD2	1:A:205:SER:HB2	2.39	0.58
4:A:604:GOL:H31	7:A:732:HOH:O	2.03	0.58
1:B:205:SER:HB3	1:B:227:LEU:HB2	1.89	0.55
1:C:121:PHE:CD2	1:C:205:SER:HB2	2.42	0.54
1:D:183:ALA:O	1:D:187:VAL:HG23	2.06	0.54
1:D:167:ASP:HB3	1:D:170:MET:HG2	1.90	0.54
1:A:115:ALA:HA	4:A:603:GOL:H2	1.90	0.54
4:C:604:GOL:H32	1:D:112:ALA:HB2	1.90	0.54
4:A:604:GOL:C3	7:A:732:HOH:O	2.55	0.53
1:D:319:GLN:NE2	7:D:705:HOH:O	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:PHE:CD2	1:B:205:SER:HB2	2.44	0.53
2:D:602:HEM:HBB2	2:D:602:HEM:CMB	2.40	0.52
1:C:182[A]:VAL:HG22	1:C:291:THR:HG21	1.90	0.52
1:D:33:VAL:HG13	1:D:37:GLY:HA3	1.93	0.51
1:B:33:VAL:HG22	1:B:40:LEU:HD21	1.93	0.50
1:A:167:ASP:HB3	1:A:170:MET:HG2	1.92	0.50
1:B:460:HIS:ND1	1:B:495:GLU:OE2	2.39	0.50
1:C:64:HIS:CE1	1:C:105:VAL:HG22	2.47	0.49
1:D:485:ASP:HA	4:D:604:GOL:H2	1.93	0.49
1:A:64:HIS:CE1	1:A:105:VAL:HG22	2.47	0.49
1:D:66:HIS:NE2	1:D:113:ASP:OD1	2.43	0.48
1:B:207:SER:HB3	1:B:225:VAL:HB	1.94	0.48
1:A:207:SER:HB3	1:A:225:VAL:HB	1.95	0.48
1:D:132:VAL:HB	1:D:331:VAL:HG13	1.96	0.48
1:D:71:PHE:CE1	1:D:99:LEU:HD13	2.49	0.47
1:D:298:GLN:OE1	1:D:298:GLN:N	2.47	0.47
1:A:98:CYS:HA	1:A:124:LYS:O	2.14	0.47
1:A:109[B]:LYS:HE2	1:A:321:GLU:OE1	2.14	0.47
1:A:359:PRO:HB3	1:C:55:ARG:HD3	1.97	0.47
1:A:476:ARG:NH1	7:A:702:HOH:O	2.33	0.47
1:D:121:PHE:CD2	1:D:205:SER:HB2	2.50	0.47
1:B:119:ARG:HG3	1:B:203:MET:HE3	1.96	0.47
1:C:205:SER:HB3	1:C:227:LEU:HB2	1.96	0.46
1:C:215:ASN:ND2	1:C:219:GLU:HG2	2.30	0.46
1:B:72:GLY:HA3	1:B:308:VAL:O	2.16	0.46
2:C:601:HEM:HMB2	2:C:601:HEM:CBB	2.42	0.46
1:B:55:ARG:HD3	1:D:359:PRO:HB3	1.97	0.46
1:D:341:VAL:HG13	2:D:602:HEM:HAB	1.97	0.46
1:B:293:VAL:HG21	3:B:602:NDP:C7N	2.46	0.45
1:B:373:LYS:HE3	1:B:373:LYS:H	1.81	0.45
1:C:341:VAL:HG13	2:C:601:HEM:HAB	1.98	0.45
1:B:132:VAL:HB	1:B:331:VAL:HG13	1.97	0.45
2:B:601:HEM:HBB2	2:B:601:HEM:HMB2	1.97	0.45
1:A:20:GLN:HG3	1:C:329:HIS:CD2	2.52	0.45
1:C:215:ASN:HD21	1:C:219:GLU:HG2	1.82	0.45
1:C:3:HIS:ND1	1:C:4:PRO:HD2	2.33	0.45
1:C:189:ILE:HG22	7:C:922:HOH:O	2.17	0.44
1:C:64:HIS:HA	1:C:104:THR:O	2.17	0.44
1:C:166:LYS:NZ	7:C:711:HOH:O	2.42	0.44
1:B:287:VAL:HG23	1:B:294:TRP:HZ2	1.83	0.44
1:D:188:MET:HG3	1:D:440:ALA:HB1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:THR:HA	1:D:268:TRP:CD1	2.52	0.44
1:D:121:PHE:CG	1:D:205:SER:HB2	2.53	0.44
1:B:20:GLN:HG3	1:D:329:HIS:CD2	2.53	0.43
1:A:72:GLY:HA3	1:A:308:VAL:O	2.18	0.43
1:C:66:HIS:NE2	1:C:113:ASP:OD1	2.50	0.43
1:D:71:PHE:CZ	1:D:99:LEU:HD13	2.54	0.43
4:A:606:GOL:H32	1:B:249:PRO:HB3	2.00	0.43
1:C:80:ILE:HG21	1:C:304:VAL:HG22	2.01	0.43
1:A:64:HIS:HA	1:A:104:THR:O	2.19	0.42
1:B:287:VAL:HG23	1:B:294:TRP:CZ2	2.53	0.42
1:A:460:HIS:ND1	1:A:495:GLU:OE2	2.49	0.42
1:C:150:PHE:HB3	1:C:151:PRO:HD3	2.02	0.42
1:A:71:PHE:HB2	1:A:311:GLU:HB3	2.00	0.42
1:A:136:ASN:HB3	1:A:206:TYR:O	2.18	0.42
1:A:183:ALA:O	1:A:187:VAL:HG23	2.20	0.42
4:A:604:GOL:H32	7:A:880:HOH:O	2.18	0.42
7:C:793:HOH:O	1:D:54:ASN:HA	2.19	0.42
1:D:136:ASN:HB3	1:D:206:TYR:O	2.20	0.41
1:D:343:GLN:HG3	7:D:709:HOH:O	2.20	0.41
1:C:167:ASP:HB3	1:C:170:MET:HG2	2.01	0.41
1:C:132:VAL:HG23	1:C:330:THR:HA	2.02	0.41
1:C:359:PRO:HG2	1:C:383:PRO:HD2	2.02	0.41
1:A:132:VAL:HB	1:A:331:VAL:HG13	2.02	0.41
1:B:167:ASP:OD1	1:B:169:ASP:HB2	2.20	0.41
1:B:71:PHE:HB2	1:B:311:GLU:HB3	2.02	0.41
1:A:109[B]:LYS:CE	1:A:321:GLU:OE1	2.69	0.40
1:A:205:SER:HB3	1:A:227:LEU:HB2	2.03	0.40
1:B:27:PRO:HB3	1:D:405:PHE:CZ	2.56	0.40
1:A:359:PRO:HG2	1:A:383:PRO:HD2	2.02	0.40
4:A:606:GOL:H31	7:A:972:HOH:O	2.21	0.40
1:A:181:GLN:C	1:A:183:ALA:N	2.75	0.40
1:A:11:ARG:HH11	1:A:11:ARG:HD2	1.79	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	504/537 (94%)	491 (97%)	13 (3%)	0	100	100
1	B	501/537 (93%)	486 (97%)	15 (3%)	0	100	100
1	C	503/537 (94%)	491 (98%)	12 (2%)	0	100	100
1	D	502/537 (94%)	489 (97%)	13 (3%)	0	100	100
All	All	2010/2148 (94%)	1957 (97%)	53 (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	439/465 (94%)	435 (99%)	4 (1%)	78	79
1	B	437/465 (94%)	433 (99%)	4 (1%)	78	79
1	C	440/465 (95%)	436 (99%)	4 (1%)	78	79
1	D	438/465 (94%)	434 (99%)	4 (1%)	78	79
All	All	1754/1860 (94%)	1738 (99%)	16 (1%)	78	79

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

Mol	Chain	Res	Type
1	A	1	MET
1	A	32	ARG
1	A	117	ASP
1	A	121	PHE
1	B	32	ARG
1	B	117	ASP
1	B	121	PHE
1	B	373	LYS

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Mol	Chain	Res	Type
1	C	32	ARG
1	C	117	ASP
1	C	121	PHE
1	C	139	THR
1	D	32	ARG
1	D	117	ASP
1	D	121	PHE
1	D	139	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 25 ligands modelled in this entry, 6 are monoatomic - leaving 19 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	NDP	D	603	-	45,52,52	1.11	3 (6%)	53,80,80	1.32	5 (9%)
4	GOL	D	605	-	5,5,5	0.69	0	5,5,5	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	HEM	C	601	1	41,50,50	1.82	10 (24%)	45,82,82	1.76	14 (31%)
4	GOL	B	603	-	5,5,5	0.64	0	5,5,5	0.77	0
4	GOL	D	604	-	5,5,5	0.79	0	5,5,5	0.96	0
3	NDP	B	602	-	45,52,52	1.16	4 (8%)	53,80,80	1.31	8 (15%)
4	GOL	A	604	-	5,5,5	0.13	0	5,5,5	0.35	0
4	GOL	A	605	-	5,5,5	0.76	0	5,5,5	0.81	0
3	NDP	A	602	-	45,52,52	1.01	2 (4%)	53,80,80	1.49	9 (16%)
2	HEM	B	601	1	41,50,50	1.43	4 (9%)	45,82,82	1.76	12 (26%)
4	GOL	C	604	-	5,5,5	0.98	0	5,5,5	1.10	1 (20%)
3	NDP	C	602	-	45,52,52	1.27	4 (8%)	53,80,80	1.24	4 (7%)
2	HEM	D	602	1	41,50,50	1.58	8 (19%)	45,82,82	1.55	12 (26%)
4	GOL	A	606	-	5,5,5	0.66	0	5,5,5	0.89	0
2	HEM	A	601	1	41,50,50	1.57	7 (17%)	45,82,82	2.01	12 (26%)
4	GOL	A	603	-	5,5,5	0.91	0	5,5,5	1.30	1 (20%)
4	GOL	A	607	-	5,5,5	0.63	0	5,5,5	0.81	0
4	GOL	C	603	-	5,5,5	0.84	0	5,5,5	1.10	0
4	GOL	A	608	-	5,5,5	0.89	0	5,5,5	1.13	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
3	NDP	D	603	-	-	4/30/77/77	0/5/5/5
4	GOL	D	605	-	-	2/4/4/4	-
2	HEM	C	601	1	-	2/12/54/54	-
4	GOL	B	603	-	-	0/4/4/4	-
4	GOL	D	604	-	-	2/4/4/4	-
3	NDP	B	602	-	-	5/30/77/77	0/5/5/5
4	GOL	A	604	-	-	0/4/4/4	-
4	GOL	A	605	-	-	2/4/4/4	-
3	NDP	A	602	-	-	5/30/77/77	0/5/5/5
2	HEM	B	601	1	-	2/12/54/54	-
4	GOL	C	604	-	-	2/4/4/4	-
3	NDP	C	602	-	-	7/30/77/77	0/5/5/5
2	HEM	D	602	1	-	2/12/54/54	-
4	GOL	A	606	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	601	1	-	4/12/54/54	-
4	GOL	A	603	-	-	1/4/4/4	-
4	GOL	A	607	-	-	2/4/4/4	-
4	GOL	C	603	-	-	0/4/4/4	-
4	GOL	A	608	-	-	2/4/4/4	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	HEM	C3C-C2C	-5.27	1.33	1.40
2	B	601	HEM	C3C-C2C	-5.26	1.33	1.40
2	D	602	HEM	C3C-C2C	-4.82	1.33	1.40
2	A	601	HEM	C3C-CAC	4.33	1.56	1.47
3	C	602	NDP	C6N-C5N	4.26	1.40	1.33
2	A	601	HEM	C3C-C2C	-3.93	1.34	1.40
2	C	601	HEM	C3C-CAC	3.68	1.55	1.47
3	B	602	NDP	C6N-C5N	3.67	1.39	1.33
3	C	602	NDP	O4B-C1B	3.57	1.46	1.41
3	D	603	NDP	C6N-C5N	3.54	1.39	1.33
3	A	602	NDP	C6N-C5N	3.52	1.39	1.33
2	C	601	HEM	CAA-C2A	3.46	1.57	1.52
2	A	601	HEM	CMB-C2B	3.39	1.58	1.50
3	D	603	NDP	O4B-C1B	3.24	1.45	1.41
2	B	601	HEM	C3C-CAC	3.12	1.54	1.47
2	C	601	HEM	FE-NB	2.92	2.11	1.96
3	C	602	NDP	P2B-O2B	2.85	1.64	1.59
3	B	602	NDP	O4B-C1B	2.65	1.44	1.41
2	D	602	HEM	CAB-C3B	2.60	1.54	1.47
2	C	601	HEM	FE-ND	2.49	2.09	1.96
2	A	601	HEM	CAA-C2A	2.49	1.55	1.52
2	A	601	HEM	C4A-NA	2.39	1.41	1.36
2	D	602	HEM	C3C-CAC	2.36	1.52	1.47
2	D	602	HEM	FE-NB	2.36	2.08	1.96
2	C	601	HEM	CAB-C3B	2.35	1.53	1.47
2	A	601	HEM	FE-NB	2.34	2.08	1.96
3	B	602	NDP	C5A-C4A	2.31	1.47	1.40
3	B	602	NDP	O4D-C1D	2.25	1.47	1.42
2	D	602	HEM	O2A-CGA	-2.22	1.23	1.30
2	A	601	HEM	O1D-CGD	2.20	1.29	1.22
2	B	601	HEM	CAB-C3B	2.19	1.53	1.47
3	A	602	NDP	O4B-C1B	2.19	1.44	1.41
2	C	601	HEM	C4D-ND	-2.18	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	602	HEM	CMD-C2D	2.12	1.55	1.50
2	D	602	HEM	CMA-C3A	2.10	1.56	1.51
3	D	603	NDP	O4D-C1D	2.05	1.46	1.42
2	B	601	HEM	CMD-C2D	2.05	1.55	1.50
3	C	602	NDP	C5A-C4A	2.04	1.46	1.40
2	D	602	HEM	C4A-NA	2.03	1.40	1.36
2	C	601	HEM	CMC-C2C	2.03	1.56	1.51
2	C	601	HEM	O1D-CGD	2.02	1.28	1.22
2	C	601	HEM	CMB-C2B	2.00	1.55	1.50

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	HEM	CHD-C1D-ND	5.23	130.11	124.43
2	A	601	HEM	C4C-CHD-C1D	5.11	129.30	122.56
2	C	601	HEM	C1B-NB-C4B	4.62	109.85	105.07
2	A	601	HEM	C4D-ND-C1D	4.44	109.66	105.07
3	A	602	NDP	N3A-C2A-N1A	-4.41	121.79	128.68
3	D	603	NDP	N3A-C2A-N1A	-4.36	121.87	128.68
3	C	602	NDP	N3A-C2A-N1A	-4.28	121.98	128.68
3	B	602	NDP	N3A-C2A-N1A	-4.05	122.35	128.68
2	A	601	HEM	CMA-C3A-C4A	-3.94	122.41	128.46
2	A	601	HEM	C4A-C3A-C2A	3.88	109.69	107.00
2	B	601	HEM	C4A-C3A-C2A	3.81	109.65	107.00
2	A	601	HEM	CAD-CBD-CGD	-3.78	105.47	113.60
3	C	602	NDP	C1B-N9A-C4A	-3.76	120.03	126.64
2	D	602	HEM	C1B-NB-C4B	3.45	108.64	105.07
3	D	603	NDP	C3D-C2D-C1D	3.40	107.88	101.43
2	A	601	HEM	C3D-C4D-ND	-3.30	106.49	110.17
2	A	601	HEM	CHD-C1D-ND	3.30	128.01	124.43
2	C	601	HEM	CAD-CBD-CGD	-3.27	106.57	113.60
2	C	601	HEM	C4D-ND-C1D	3.26	108.44	105.07
2	C	601	HEM	C4A-C3A-C2A	3.20	109.22	107.00
3	A	602	NDP	C3N-C7N-N7N	3.18	123.32	117.67
2	C	601	HEM	C3B-C2B-C1B	3.06	108.76	106.49
3	B	602	NDP	C3D-C2D-C1D	2.99	107.11	101.43
2	A	601	HEM	C2D-C1D-ND	-2.96	106.34	109.88
3	A	602	NDP	O3X-P2B-O2X	2.91	118.78	107.64
3	A	602	NDP	C1B-N9A-C4A	-2.91	121.52	126.64
2	D	602	HEM	CBA-CAA-C2A	-2.89	107.69	112.62
2	C	601	HEM	C4C-CHD-C1D	2.89	126.37	122.56
2	B	601	HEM	C1B-NB-C4B	2.88	108.05	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	602	HEM	C2C-C3C-C4C	2.83	108.87	106.90
2	B	601	HEM	C4D-ND-C1D	2.69	107.85	105.07
3	D	603	NDP	C1B-N9A-C4A	-2.69	121.92	126.64
3	A	602	NDP	O4D-C1D-N1N	2.60	113.14	108.06
2	B	601	HEM	C4C-CHD-C1D	2.59	125.97	122.56
2	A	601	HEM	C1D-C2D-C3D	2.55	109.64	106.96
2	B	601	HEM	CAD-CBD-CGD	-2.54	108.13	113.60
2	C	601	HEM	C2B-C1B-NB	-2.53	106.84	109.84
2	B	601	HEM	CAA-CBA-CGA	-2.52	106.70	113.76
2	C	601	HEM	CHD-C1D-C2D	2.45	128.80	124.98
2	D	602	HEM	CAD-CBD-CGD	-2.44	108.35	113.60
2	A	601	HEM	C4B-C3B-C2B	2.40	109.02	107.11
3	C	602	NDP	O4D-C1D-N1N	2.39	112.73	108.06
2	D	602	HEM	C3D-C4D-ND	-2.36	107.54	110.17
2	D	602	HEM	C4B-CHC-C1C	2.35	125.66	122.56
2	B	601	HEM	CHD-C1D-C2D	-2.34	121.32	124.98
3	D	603	NDP	O4D-C1D-N1N	2.30	112.56	108.06
2	C	601	HEM	C2D-C1D-ND	-2.29	107.14	109.88
3	A	602	NDP	O4B-C1B-C2B	2.27	110.53	106.59
3	B	602	NDP	PN-O3-PA	-2.27	125.05	132.83
2	B	601	HEM	CAD-C3D-C2D	-2.25	123.69	127.88
3	A	602	NDP	PN-O3-PA	-2.24	125.12	132.83
3	B	602	NDP	C1B-N9A-C4A	-2.24	122.71	126.64
3	B	602	NDP	C2A-N1A-C6A	2.21	122.54	118.75
2	A	601	HEM	CHC-C4B-C3B	2.21	127.96	124.57
2	C	601	HEM	CMC-C2C-C3C	2.21	128.81	124.68
3	D	603	NDP	C2A-N1A-C6A	2.21	122.53	118.75
2	A	601	HEM	CHA-C4D-C3D	2.20	129.46	125.33
2	B	601	HEM	O2D-CGD-CBD	2.18	121.04	114.03
3	B	602	NDP	N6A-C6A-N1A	2.17	123.08	118.57
2	D	602	HEM	CAA-CBA-CGA	-2.16	107.71	113.76
3	C	602	NDP	C2B-C3B-C4B	2.15	106.66	101.99
2	B	601	HEM	CHB-C1B-NB	2.14	127.03	124.38
4	A	603	GOL	C3-C2-C1	-2.14	103.39	111.70
3	B	602	NDP	O7N-C7N-C3N	-2.13	116.89	120.90
3	A	602	NDP	C2D-C1D-N1N	-2.11	108.02	113.30
2	C	601	HEM	CHC-C4B-C3B	2.07	127.73	124.57
2	D	602	HEM	C2B-C1B-NB	-2.06	107.39	109.84
2	C	601	HEM	O1D-CGD-CBD	-2.06	116.47	123.08
3	B	602	NDP	O2N-PN-O1N	2.05	122.38	112.24
2	D	602	HEM	C3C-C4C-NC	-2.05	107.08	110.94
2	D	602	HEM	C3B-C2B-C1B	2.05	108.00	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	602	HEM	C4D-ND-C1D	2.04	107.18	105.07
4	C	604	GOL	C3-C2-C1	-2.03	103.81	111.70
2	C	601	HEM	O2D-CGD-CBD	2.02	120.53	114.03
2	D	602	HEM	CMA-C3A-C4A	-2.02	125.36	128.46
2	C	601	HEM	C3D-C4D-ND	-2.01	107.93	110.17
3	A	602	NDP	O2N-PN-O1N	2.00	122.15	112.24
2	B	601	HEM	CMC-C2C-C3C	2.00	128.42	124.68

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	NDP	C2B-O2B-P2B-O2X
3	B	602	NDP	C5B-O5B-PA-O3
3	B	602	NDP	C3B-C4B-C5B-O5B
3	C	602	NDP	O4B-C4B-C5B-O5B
3	D	603	NDP	C2N-C3N-C7N-N7N
4	A	607	GOL	C1-C2-C3-O3
4	A	607	GOL	O2-C2-C3-O3
4	A	608	GOL	C1-C2-C3-O3
4	A	608	GOL	O2-C2-C3-O3
4	D	604	GOL	O1-C1-C2-C3
3	A	602	NDP	O4B-C4B-C5B-O5B
3	C	602	NDP	C3B-C4B-C5B-O5B
4	A	605	GOL	O1-C1-C2-C3
4	C	604	GOL	O1-C1-C2-C3
4	D	605	GOL	O1-C1-C2-C3
4	A	605	GOL	O1-C1-C2-O2
4	C	604	GOL	O1-C1-C2-O2
4	D	604	GOL	O1-C1-C2-O2
4	D	605	GOL	O1-C1-C2-O2
3	B	602	NDP	O4B-C4B-C5B-O5B
4	A	603	GOL	O1-C1-C2-O2
3	A	602	NDP	O4D-C1D-N1N-C6N
3	C	602	NDP	C2B-O2B-P2B-O2X
3	C	602	NDP	PA-O3-PN-O1N
3	C	602	NDP	O4D-C1D-N1N-C6N
3	B	602	NDP	C5B-O5B-PA-O2A
3	C	602	NDP	C5B-O5B-PA-O1A
3	D	603	NDP	O4D-C1D-N1N-C6N
3	B	602	NDP	O4D-C1D-N1N-C6N
3	A	602	NDP	C3B-C4B-C5B-O5B

Continued on next page...

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Mol	Chain	Res	Type	Atoms
3	D	603	NDP	O4B-C4B-C5B-O5B
2	A	601	HEM	CAD-CBD-CGD-O2D
2	C	601	HEM	CAD-CBD-CGD-O2D
2	D	602	HEM	CAD-CBD-CGD-O2D
2	B	601	HEM	CAD-CBD-CGD-O2D
3	A	602	NDP	C2B-O2B-P2B-O1X
2	C	601	HEM	CAD-CBD-CGD-O1D
2	A	601	HEM	CAA-CBA-CGA-O1A
2	B	601	HEM	CAD-CBD-CGD-O1D
2	D	602	HEM	CAD-CBD-CGD-O1D
2	A	601	HEM	CAA-CBA-CGA-O2A
2	A	601	HEM	CAD-CBD-CGD-O1D
3	C	602	NDP	PA-O3-PN-O2N
3	D	603	NDP	PA-O3-PN-O2N

There are no ring outliers.

10 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	HEM	4	0
4	D	604	GOL	1	0
3	B	602	NDP	1	0
4	A	604	GOL	3	0
2	B	601	HEM	1	0
4	C	604	GOL	1	0
2	D	602	HEM	3	0
4	A	606	GOL	2	0
2	A	601	HEM	2	0
4	A	603	GOL	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.
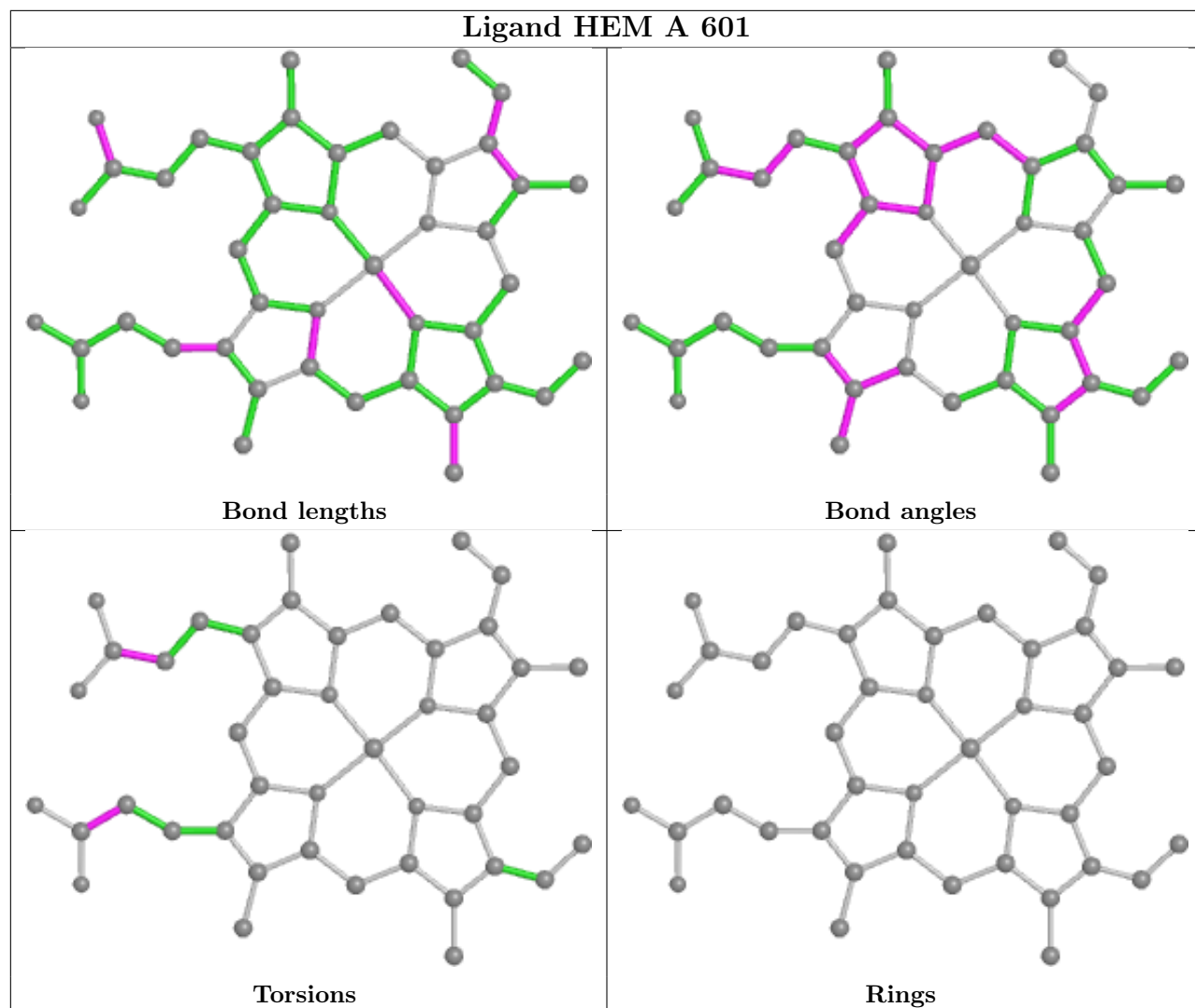
Ligand NDP D 603

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM C 601

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP B 602

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP A 602

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 601

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP C 602

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM D 602

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 601

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	505/537 (94%)	-0.41	3 (0%)	89	90	14, 25, 44, 96	0
1	B	501/537 (93%)	-0.02	9 (1%)	68	71	16, 36, 58, 96	0
1	C	500/537 (93%)	-0.37	2 (0%)	92	93	15, 26, 55, 74	0
1	D	502/537 (93%)	-0.30	4 (0%)	86	87	13, 27, 50, 73	0
All	All	2008/2148 (93%)	-0.28	18 (0%)	84	85	13, 28, 54, 96	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	3.9
1	D	2	GLY	3.7
1	B	357	LEU	2.8
1	B	59	PRO	2.8
1	B	324	ALA	2.7
1	C	4	PRO	2.4
1	C	91	THR	2.4
1	A	58	ILE	2.4
1	B	58	ILE	2.4
1	B	297	LYS	2.2
1	B	486	ARG	2.2
1	D	78	ASP	2.2
1	A	-2	GLN	2.2
1	B	485	ASP	2.2
1	B	352	ALA	2.1
1	B	361	TYR	2.0
1	D	503	LYS	2.0
1	D	91	THR	2.0

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

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

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
4	GOL	A	608	6/6	0.81	0.26	68,72,75,83	0
4	GOL	D	604	6/6	0.81	0.27	73,77,85,92	0
4	GOL	A	604	6/6	0.85	0.21	59,63,66,80	0
4	GOL	B	603	6/6	0.90	0.20	58,65,74,75	0
4	GOL	A	607	6/6	0.91	0.25	30,77,80,84	0
4	GOL	A	603	6/6	0.91	0.18	46,58,84,87	0
4	GOL	A	605	6/6	0.92	0.18	54,61,64,68	0
4	GOL	D	605	6/6	0.92	0.15	40,49,57,61	0
5	K	B	604	1/1	0.92	0.10	72,72,72,72	0
4	GOL	C	604	6/6	0.93	0.15	51,55,65,68	0
4	GOL	C	603	6/6	0.93	0.17	45,59,63,86	0
3	NDP	B	602	48/48	0.94	0.14	44,56,65,79	0
4	GOL	A	606	6/6	0.95	0.22	62,73,81,85	0
3	NDP	C	602	48/48	0.97	0.08	24,29,44,55	0
5	K	A	609	1/1	0.97	0.08	48,48,48,48	0
3	NDP	D	603	48/48	0.97	0.07	23,33,49,64	0
6	CL	D	601	1/1	0.97	0.06	34,34,34,34	0
2	HEM	C	601	43/43	0.98	0.10	10,16,27,40	0
2	HEM	D	602	43/43	0.98	0.11	15,18,26,32	0
3	NDP	A	602	48/48	0.98	0.06	18,25,34,43	0
2	HEM	A	601	43/43	0.98	0.15	10,14,25,35	0
5	K	C	605	1/1	0.98	0.08	46,46,46,46	0
5	K	D	606	1/1	0.98	0.06	53,53,53,53	0
6	CL	B	605	1/1	0.98	0.07	37,37,37,37	0
2	HEM	B	601	43/43	0.98	0.15	17,22,35,48	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.
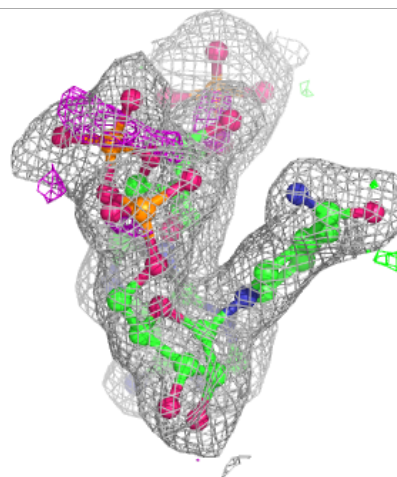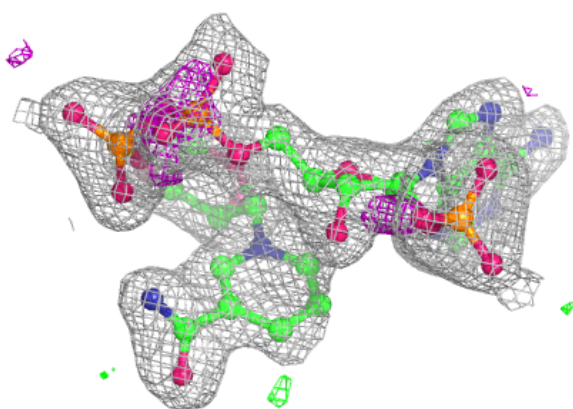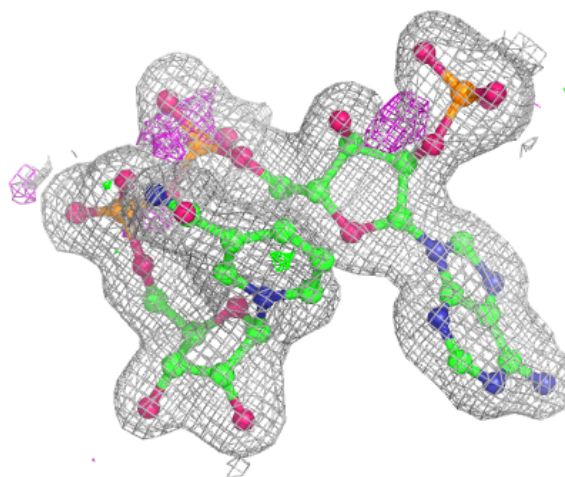
Electron density around NDP B 602:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
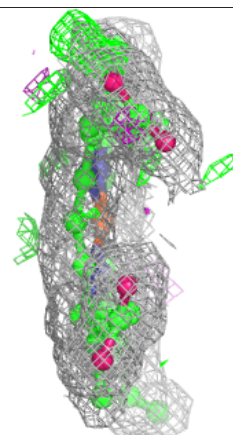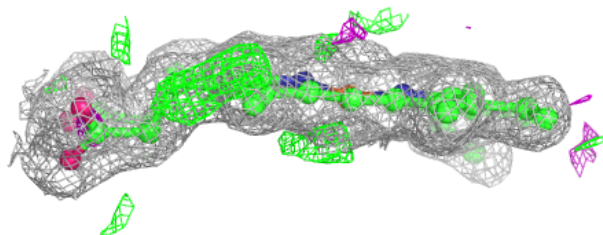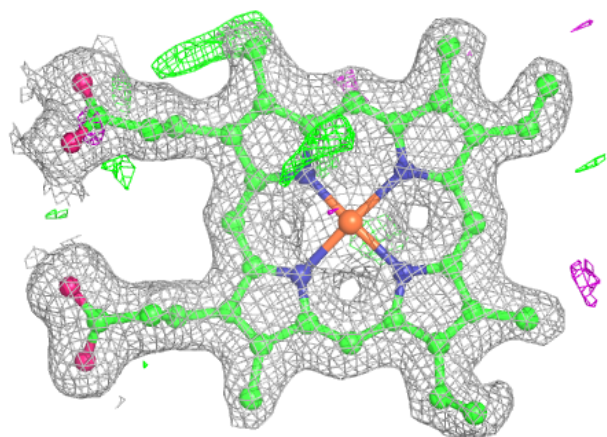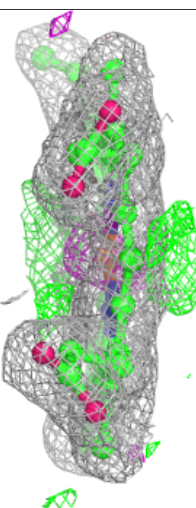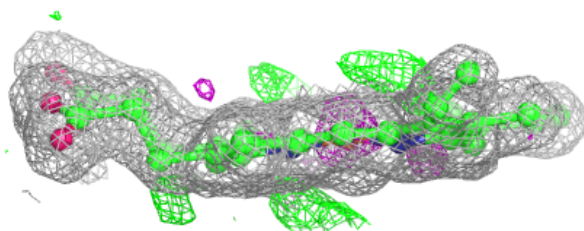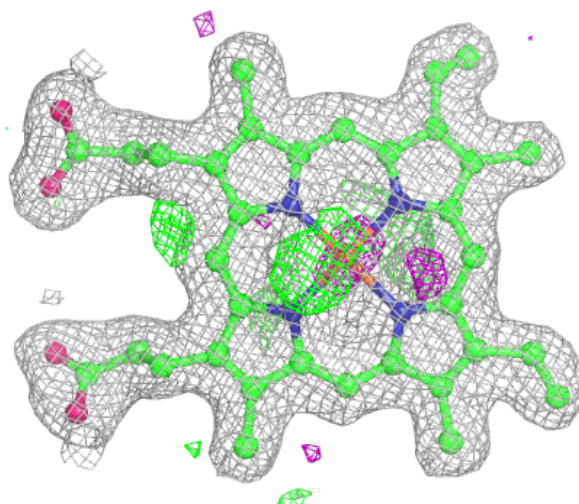$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
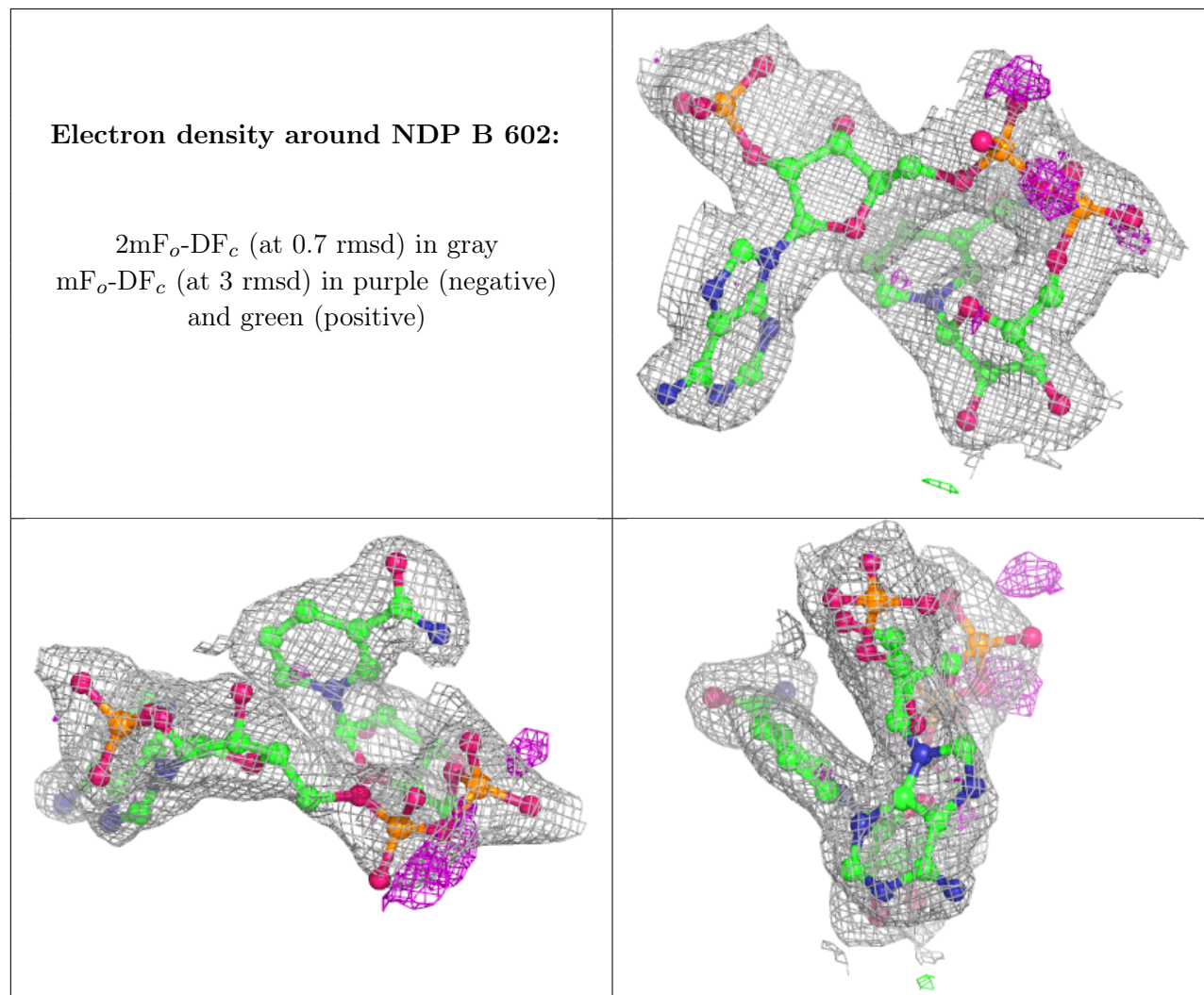
Electron density around NDP C 602:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
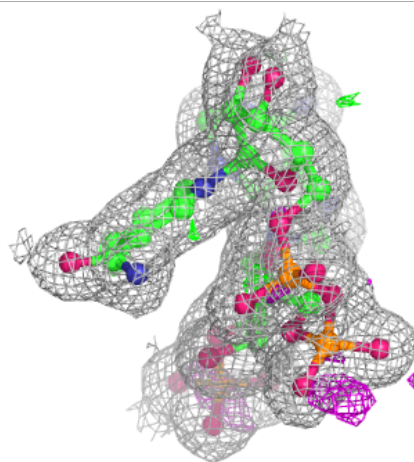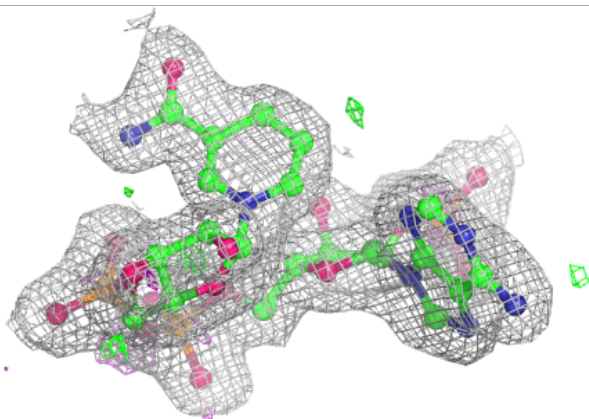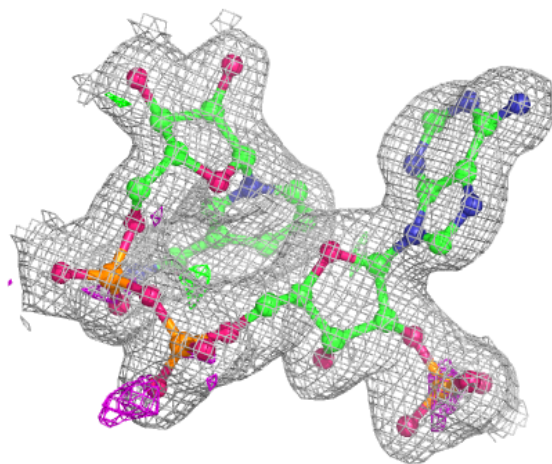and green (positive)
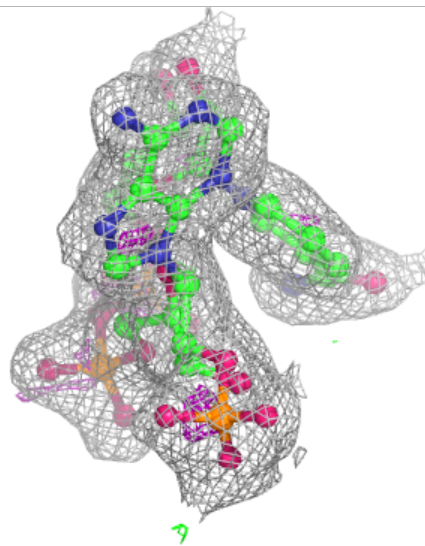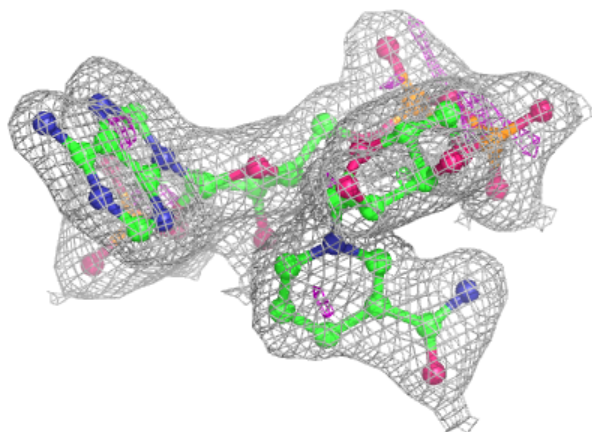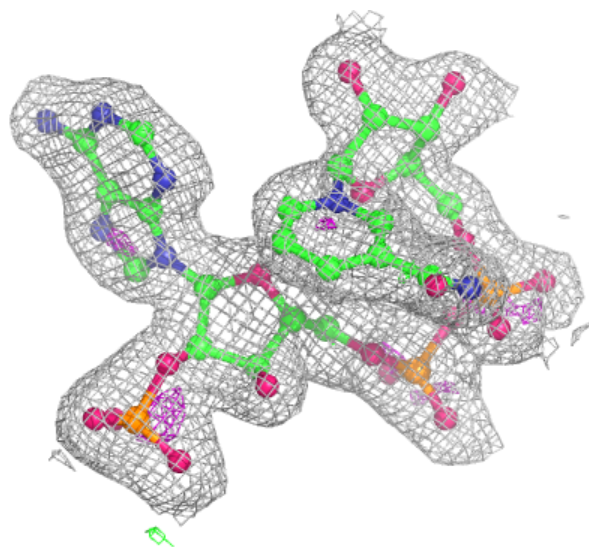
Electron density around NDP D 603:

$2mF_o$-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 C 601:

$2mF_o\text{-}DF_c$ (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 602:

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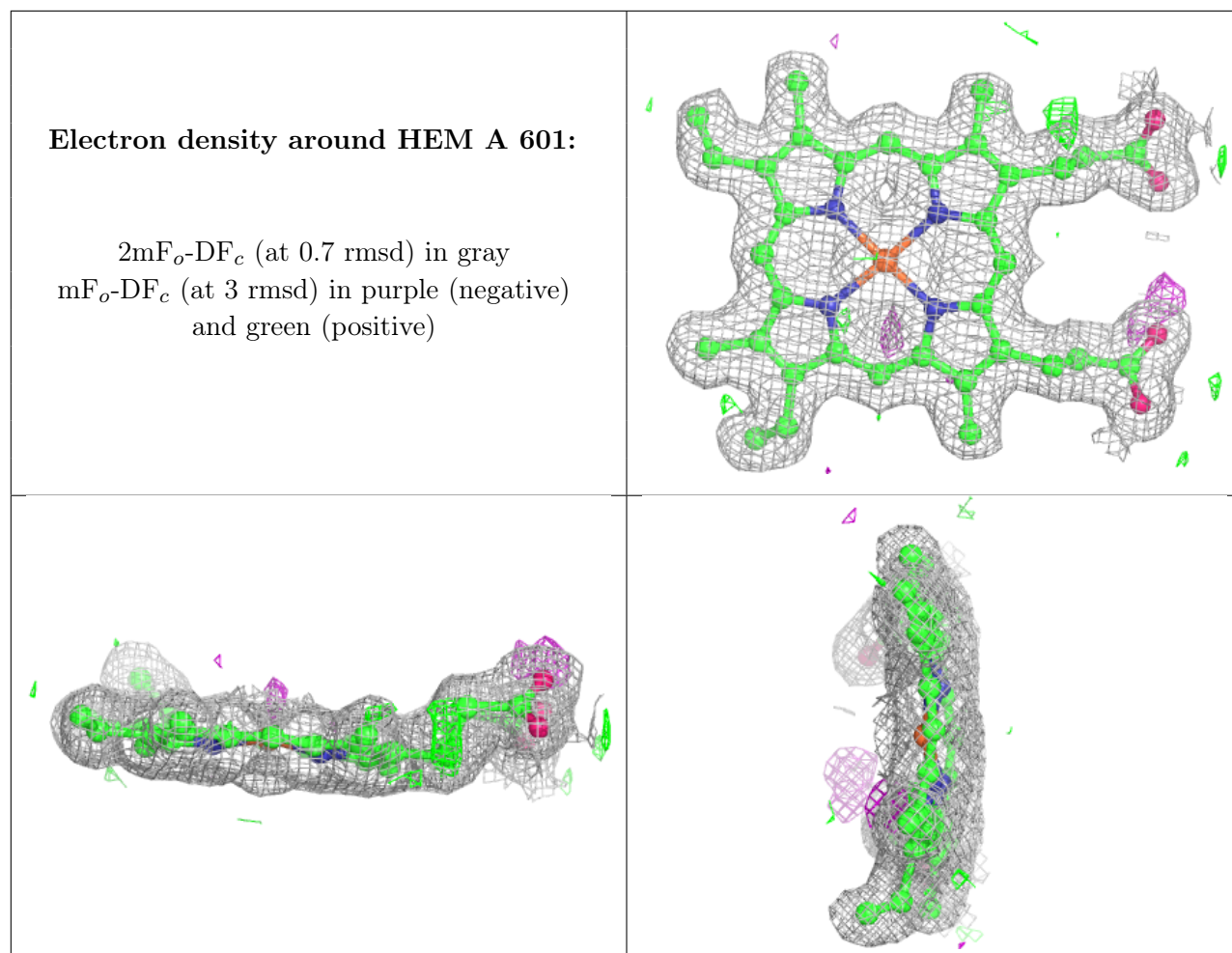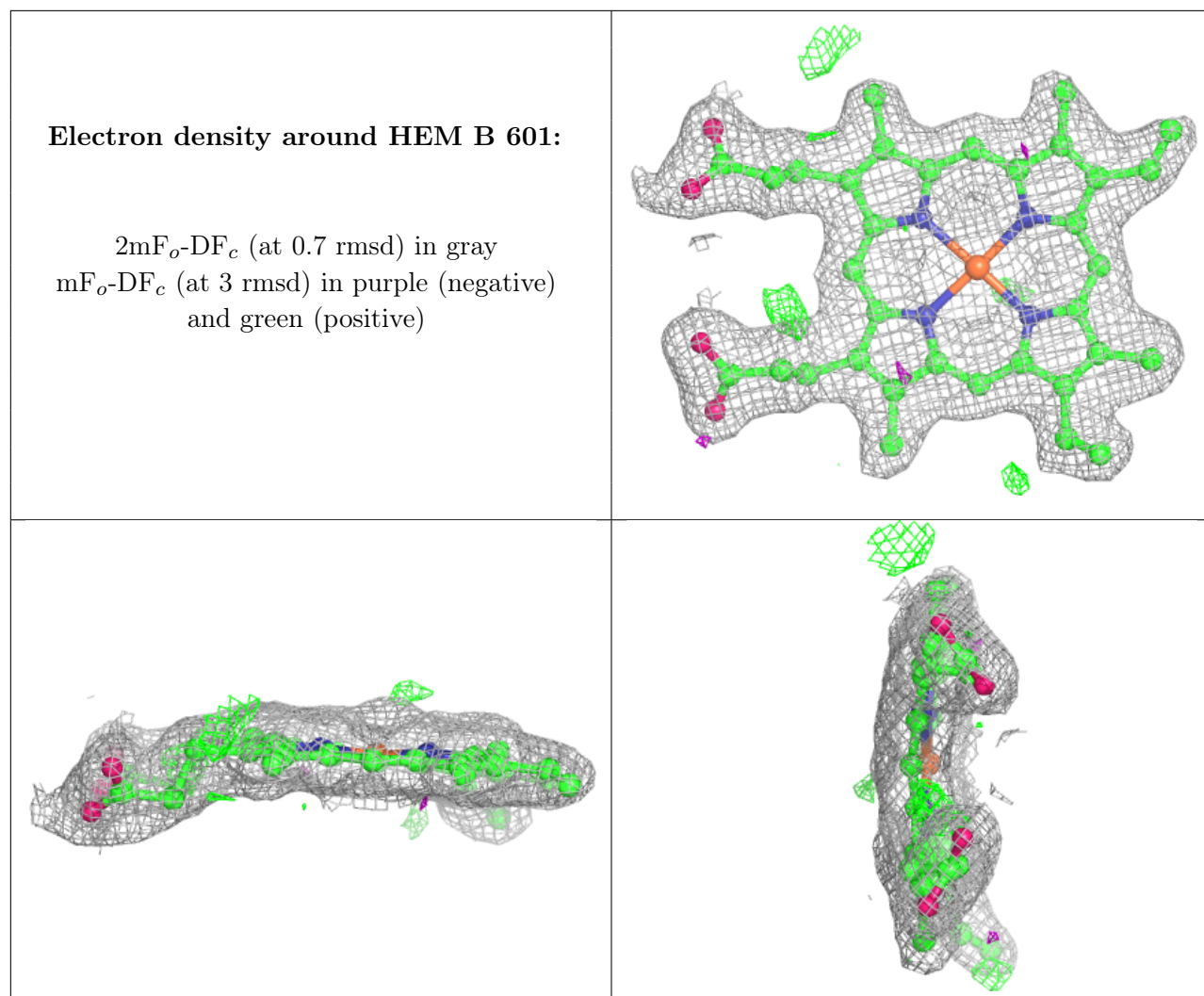mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around NDP A 602:

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

Electron density around HEM A 601:

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

Electron density around HEM B 601:

$2mF_o$-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.