Full wwPDB X-ray Structure Validation Report (i)

Aug 2, 2023 – 04:58 AM EDT

PDB ID	:	1DGH
Title	:	HUMAN ERYTHROCYTE CATALASE 3-AMINO-1,2,4-TRIAZOLE COMPLEX
Authors	:	Putnam, C.D.; Arvai, A.S.; Bourne, Y.; Tainer, J.A.
Deposited on	:	1999-11-24
Resolution	:	2.00 Å(reported)

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

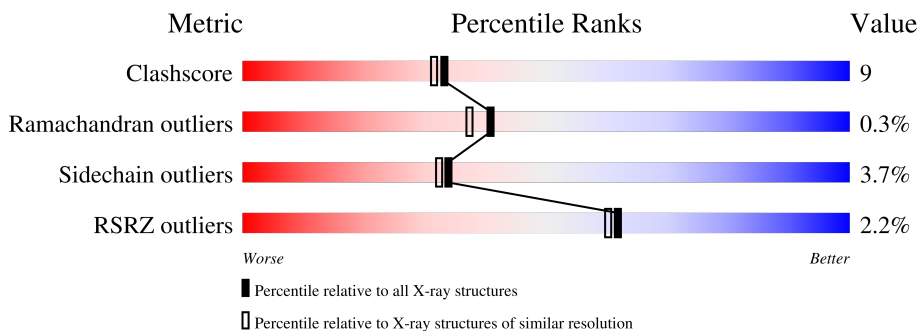|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1   Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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
Clashscore		9
Ramachandran outliers		0.3%
Sidechain outliers		3.7%
RSRZ outliers		2.2%

Worse .... *Better*

▌ 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	498	2% · 84% · 14% ·
1	C	498	2% · 82% · 17% ·
2	B	498	2% · 81% · 17% ·
2	D	498	2% · 86% · 13% ·

2   Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 17815 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 PROTEIN (CATALASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	2	0
			4012	2548	712	739	13			
1	C	498	Total	C	N	O	S	0	2	0
			4018	2551	713	741	13			

- Molecule 2 is a protein called PROTEIN (CATALASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	498	Total	C	N	O	S	0	2	0
			4024	2553	717	741	13			
2	D	498	Total	C	N	O	S	0	2	0
			4024	2553	717	741	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	75	3AH	HIS	modified residue	UNP P04040
D	75	3AH	HIS	modified residue	UNP P04040

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

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

- Molecule 4 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
4	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
4	C	1	Total 48	C 21	N 7	O 17	P 3	0	0

• Molecule 5 is water.

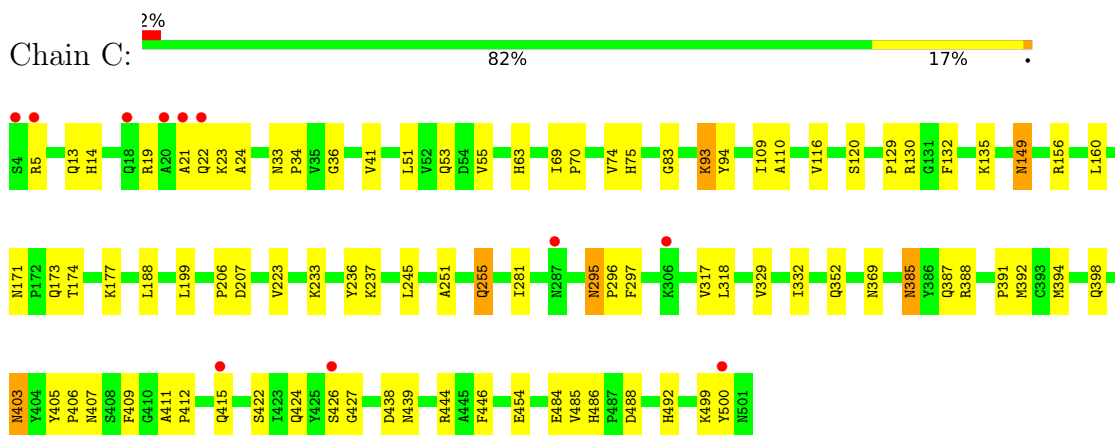| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	380	Total 380	O 380	0	0
5	B	357	Total 357	O 357	0	0
5	C	384	Total 384	O 384	0	0
5	D	348	Total 348	O 348	0	0

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.
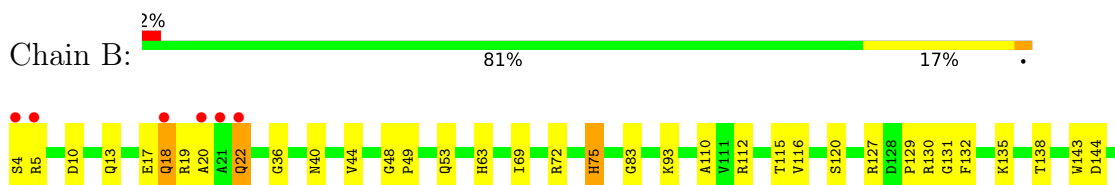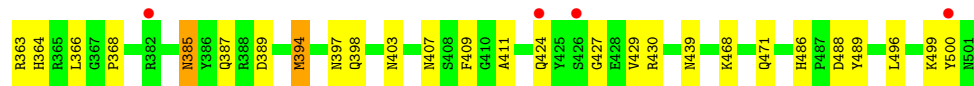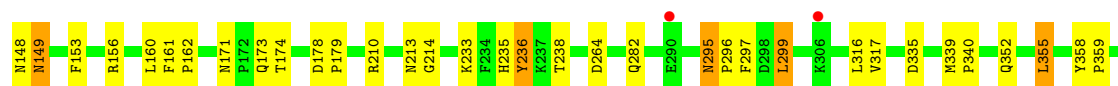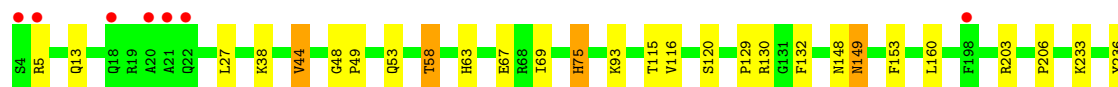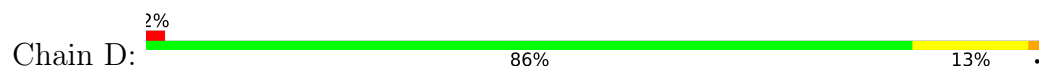
• Molecule 1: PROTEIN (CATALASE)
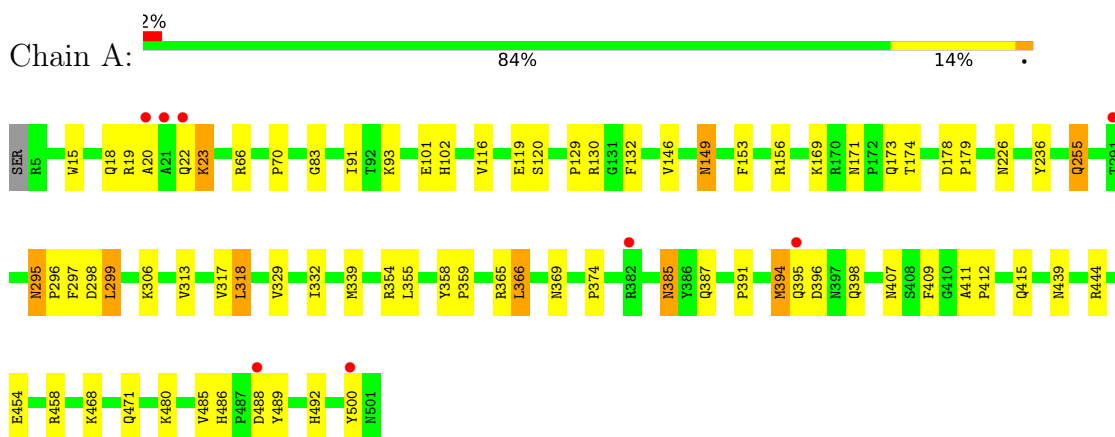
• Molecule 1: PROTEIN (CATALASE)

• Molecule 2: PROTEIN (CATALASE)

N148 N149 F153 R156 L160 F161 P162 N171 P172 Q173 T174 D178 P179 R210 N213 G214 K233 F234 H235 Y236 K237 T238 D264 Q282 E290 N295 P296 F297 D298 L299 K306 L316 V317 D335 M339 P340 Q352 L355 Y358 P359

R363 H364 R365 L366 G367 P368 R382 N385 Y386 Q387 R388 D389 M394 N397 Q398 N403 N407 S408 F409 G410 A411 Q424 Y425 S426 G427 E428 V429 R430 N439 K468 Q471 H486 P487 D488 Y489 L496 K499 Y500 N501

• Molecule 2: PROTEIN (CATALASE)

Chain D:

2%

86%   13%   •

S4 R5 Q13 Q18 R19 A20 A21 Q22 L27 K38 V44 G48 P49 Q53 T58 H63 E67 R68 I69 H75 K93 T115 V116 S120 P129 R130 G131 F132 N148 N149 F153 L160 F198 R203 P206 K233 Y236

I242 E248 Q255 P275 Q282 T285 Q288 F292 P293 F294 N295 P296 F297 D298 K306 L318 F334 M339 Q352 P359 H362 N369 P374 R380 A381 R382 N385 Y386 Q387 P391 M394 Q398 N403 N407 S408 F409

G410 A411 P412 Q415 P416 L419 N433 R444 K457 E461 Q471 V485 H486 P487 D488 Y489 K499 Y500 N501

4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.03Å 140.64Å 231.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.99 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.00) 93.8 (19.99-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	0.74 (at 2.01Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.173 , 0.210 0.170 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	42.4	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.9	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	17815	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: HEM, 3AH, 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	0.34	0/4131	0.62	0/5611
1	C	0.35	0/4137	0.63	0/5619
2	B	0.35	0/4125	0.63	0/5601
2	D	0.35	0/4125	0.62	0/5601
All	All	0.35	0/16518	0.62	0/22432

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 ⓘ

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	4012	0	3840	68	0
1	C	4018	0	3845	87	0
2	B	4024	0	3846	88	0
2	D	4024	0	3846	79	0
3	A	43	0	30	0	0
3	B	43	0	30	1	0
3	C	43	0	30	0	0
3	D	43	0	30	0	0
4	A	48	0	26	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	48	0	26	1	0
5	A	380	0	0	6	0
5	B	357	0	0	6	0
5	C	384	0	0	11	0
5	D	348	0	0	10	0
All	All	17815	0	15549	275	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 9.

All (275) 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:D:382:ARG:H	2:D:382:ARG:HD3	1.07	1.14
2:B:13:GLN:HG2	2:D:471:GLN:HE22	1.36	0.90
2:B:156:ARG:HH12	2:B:439:ASN:HD21	1.18	0.90
1:A:156:ARG:HH22	1:A:439:ASN:HD21	1.21	0.88
1:A:407:ASN:HD22	1:A:409:PHE:H	1.20	0.88
2:B:385:ASN:H	2:B:398:GLN:HE22	1.23	0.87
2:B:424:GLN:HE21	1:C:427:GLY:H	1.21	0.87
2:B:120[B]:SER:O	2:D:120[B]:SER:O	1.93	0.86
2:B:471:GLN:HE22	2:D:13:GLN:HE21	1.19	0.86
1:C:156:ARG:HH12	1:C:439:ASN:HD21	1.21	0.84
2:D:382:ARG:HD3	2:D:382:ARG:N	1.91	0.84
2:D:486:HIS:HD2	2:D:488:ASP:H	1.24	0.84
1:C:385:ASN:H	1:C:398:GLN:HE22	1.23	0.84
1:C:63:HIS:HE1	2:D:369:ASN:HD21	1.27	0.83
1:A:156:ARG:HH12	1:A:439:ASN:HD22	1.22	0.83
1:C:34:PRO:HG3	2:D:382:ARG:HH22	1.45	0.82
1:A:385:ASN:H	1:A:398:GLN:HE22	1.23	0.81
2:D:116:VAL:HG21	2:D:129:PRO:HG2	1.62	0.80
1:C:352:GLN:HE22	2:D:53:GLN:HE21	1.30	0.79
2:D:385:ASN:H	2:D:398:GLN:HE22	1.30	0.79
2:D:382:ARG:H	2:D:382:ARG:CD	1.94	0.79
1:A:369:ASN:HD21	2:B:63:HIS:HE1	1.30	0.78
1:C:369:ASN:HD21	2:D:63:HIS:HE1	1.29	0.78
1:A:156:ARG:HH12	1:A:439:ASN:ND2	1.82	0.77
2:B:116:VAL:HG21	2:B:129:PRO:HG2	1.66	0.77
2:B:424:GLN:NE2	1:C:427:GLY:H	1.83	0.77
1:A:454:GLU:HB3	1:A:458:ARG:HH21	1.48	0.77
2:D:407:ASN:HD22	2:D:409:PHE:H	1.30	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:MET:HG2	2:D:394:MET:HG3	1.66	0.76
1:C:369:ASN:ND2	2:D:63:HIS:HE1	1.83	0.76
2:B:49:PRO:HB2	1:C:51:LEU:HD23	1.66	0.76
1:C:392:MET:HB3	1:C:394:MET:HE1	1.68	0.75
1:C:156:ARG:HH22	1:C:439:ASN:HD22	1.33	0.74
2:B:13:GLN:HG2	2:D:471:GLN:NE2	2.01	0.74
1:A:395:GLN:HG3	1:A:396:ASP:H	1.50	0.74
5:C:3380:HOH:O	2:D:382:ARG:HG2	1.87	0.74
1:A:22:GLN:O	1:A:23:LYS:HB3	1.87	0.73
2:B:75:3AH:N2	2:B:148:ASN:HB3	2.04	0.72
1:A:171:ASN:ND2	1:A:173:GLN:H	1.87	0.72
1:A:130:ARG:H	1:A:149:ASN:ND2	1.88	0.71
1:A:116:VAL:HG21	1:A:129:PRO:HG2	1.72	0.71
2:D:58:THR:HG21	5:D:2075:HOH:O	1.90	0.71
1:C:63:HIS:HE1	2:D:369:ASN:ND2	1.88	0.70
1:C:171:ASN:ND2	1:C:173:GLN:H	1.89	0.70
1:C:407:ASN:HD22	1:C:409:PHE:H	1.40	0.70
1:C:486:HIS:HD2	1:C:488:ASP:H	1.37	0.70
2:B:156:ARG:HH22	2:B:439:ASN:HD22	1.38	0.70
2:B:171:ASN:ND2	2:B:173:GLN:H	1.89	0.70
1:C:116:VAL:HG21	1:C:129:PRO:HG2	1.74	0.69
2:B:471:GLN:HE22	2:D:13:GLN:NE2	1.91	0.68
1:A:486:HIS:HD2	1:A:488:ASP:HB3	1.60	0.67
1:C:149:ASN:H	1:C:149:ASN:HD22	1.43	0.66
1:C:171:ASN:HD22	1:C:174:THR:H	1.41	0.66
1:A:15:TRP:O	1:A:18:GLN:HG2	1.95	0.65
1:A:120[B]:SER:O	1:C:120[B]:SER:O	2.13	0.65
2:B:427:GLY:H	1:C:424:GLN:HE21	1.42	0.65
1:C:295:ASN:ND2	1:C:297:PHE:H	1.94	0.65
1:C:34:PRO:HG3	2:D:382:ARG:NH2	2.12	0.65
1:A:369:ASN:ND2	2:B:63:HIS:HE1	1.94	0.65
2:D:486:HIS:CD2	2:D:488:ASP:H	2.13	0.65
2:B:427:GLY:H	1:C:424:GLN:NE2	1.93	0.65
1:C:63:HIS:HD2	5:C:3032:HOH:O	1.80	0.65
2:D:444:ARG:HD3	2:D:485:VAL:O	1.96	0.65
1:C:53:GLN:HE21	2:D:352:GLN:HE22	1.44	0.64
1:A:149:ASN:H	1:A:149:ASN:HD22	1.44	0.64
1:A:394:MET:HE2	2:B:394:MET:HB2	1.78	0.64
2:B:149:ASN:HD22	2:B:149:ASN:H	1.44	0.64
2:D:381:ALA:HB1	2:D:382:ARG:HH11	1.63	0.64
2:D:457:LYS:O	2:D:461:GLU:HG2	1.96	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:424:GLN:HE21	1:C:427:GLY:N	1.95	0.63
1:C:156:ARG:HH22	1:C:439:ASN:ND2	1.97	0.62
1:A:486:HIS:CD2	1:A:488:ASP:HB3	2.34	0.62
2:D:130:ARG:H	2:D:149:ASN:ND2	1.96	0.62
2:B:153:PHE:HB3	2:B:299:LEU:HD13	1.80	0.62
1:C:369:ASN:HD21	2:D:63:HIS:CE1	2.15	0.62
2:D:380:ARG:HB3	2:D:380:ARG:HH11	1.65	0.62
2:D:486:HIS:CD2	2:D:488:ASP:HB3	2.35	0.61
1:A:471:GLN:NE2	1:C:13:GLN:HG2	2.16	0.61
1:A:171:ASN:HD22	1:A:173:GLN:H	1.49	0.60
2:B:171:ASN:HD22	2:B:174:THR:H	1.47	0.60
2:B:407:ASN:HD22	2:B:409:PHE:H	1.50	0.60
1:C:352:GLN:NE2	2:D:53:GLN:HE21	1.99	0.60
2:D:75:3AH:HN32	2:D:153:PHE:HE2	1.50	0.60
1:A:471:GLN:HE22	1:C:13:GLN:HG2	1.66	0.59
2:B:171:ASN:HD22	2:B:173:GLN:H	1.49	0.59
2:B:156:ARG:HH22	2:B:439:ASN:ND2	2.00	0.59
1:A:480:LYS:HA	5:A:3350:HOH:O	2.03	0.58
1:C:486:HIS:CD2	1:C:488:ASP:H	2.20	0.58
2:D:380:ARG:HH11	2:D:380:ARG:CB	2.17	0.58
1:A:339:MET:HE2	5:A:3330:HOH:O	2.04	0.57
1:C:130:ARG:H	1:C:149:ASN:ND2	2.03	0.57
1:C:149:ASN:HD22	1:C:149:ASN:N	2.02	0.57
2:D:75:3AH:N2	2:D:148:ASN:HB3	2.20	0.57
2:B:149:ASN:HD22	2:B:149:ASN:N	2.01	0.57
2:B:130:ARG:H	2:B:149:ASN:ND2	2.03	0.57
1:C:329:VAL:O	1:C:332:ILE:HG22	2.05	0.57
2:B:295:ASN:HD22	2:B:296:PRO:HD2	1.69	0.56
2:D:75:3AH:HN31	2:D:148:ASN:ND2	2.03	0.56
2:B:153:PHE:CB	2:B:299:LEU:HD13	2.35	0.56
1:A:169:LYS:HB3	5:A:3146:HOH:O	2.06	0.56
2:B:63:HIS:HD2	5:B:2013:HOH:O	1.88	0.56
2:B:496:LEU:O	2:B:499:LYS:HG2	2.06	0.56
1:C:171:ASN:ND2	1:C:174:THR:H	2.03	0.55
1:C:237:LYS:HE2	5:C:3322:HOH:O	2.07	0.55
1:C:171:ASN:HD22	1:C:173:GLN:H	1.55	0.55
2:B:486:HIS:HD2	2:B:488:ASP:H	1.54	0.55
2:B:156:ARG:HH12	2:B:439:ASN:ND2	1.99	0.54
1:C:63:HIS:CE1	2:D:369:ASN:HD21	2.16	0.54
2:B:17:GLU:C	2:B:19:ARG:H	2.10	0.54
2:B:389:ASP:H	2:B:397:ASN:HD21	1.54	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ARG:NH2	1:A:439:ASN:HD21	1.99	0.53
1:C:83:GLY:HA3	1:C:317:VAL:O	2.08	0.53
2:D:149:ASN:HD22	2:D:149:ASN:H	1.56	0.53
2:B:53:GLN:HB2	5:C:3018:HOH:O	2.07	0.53
2:D:44:VAL:CG1	2:D:49:PRO:HD2	2.38	0.53
2:D:295:ASN:ND2	2:D:297:PHE:H	2.07	0.52
2:B:385:ASN:ND2	2:B:387:GLN:H	2.08	0.51
2:D:380:ARG:HH11	2:D:380:ARG:CG	2.23	0.51
2:B:127:ARG:NH1	5:B:2274:HOH:O	2.38	0.51
1:A:295:ASN:HD22	1:A:296:PRO:HD2	1.75	0.51
2:D:295:ASN:HB3	2:D:298:ASP:HB2	1.92	0.51
2:B:352:GLN:HA	2:B:355:LEU:HD22	1.93	0.50
2:D:63:HIS:HD2	5:D:2038:HOH:O	1.92	0.50
2:B:19:ARG:HB2	2:B:22:GLN:NE2	2.26	0.50
2:D:385:ASN:ND2	2:D:387:GLN:H	2.09	0.50
2:D:44:VAL:O	2:D:48:GLY:HA3	2.10	0.50
2:D:416:PRO:O	2:D:419:LEU:HB2	2.11	0.50
2:B:161:PHE:HB3	2:B:162:PRO:HD3	1.93	0.50
1:C:484:GLU:HG3	5:C:3349:HOH:O	2.12	0.50
2:D:419:LEU:HD12	5:D:2224:HOH:O	2.11	0.50
2:D:486:HIS:HD2	2:D:488:ASP:N	2.01	0.50
2:B:156:ARG:NH1	2:B:439:ASN:HD21	1.99	0.50
2:D:203:ARG:NH1	2:D:242:ILE:HD13	2.27	0.49
2:D:381:ALA:HB1	2:D:382:ARG:NH1	2.27	0.49
2:B:171:ASN:ND2	2:B:174:THR:H	2.09	0.49
1:A:171:ASN:HD22	1:A:174:THR:H	1.60	0.49
2:B:44:VAL:O	2:B:48:GLY:HA3	2.12	0.49
2:D:285:THR:OG1	2:D:288:GLN:HG3	2.12	0.49
2:D:44:VAL:HG13	2:D:49:PRO:HD2	1.95	0.49
1:A:385:ASN:ND2	1:A:387:GLN:H	2.11	0.49
1:C:21:ALA:O	1:C:23:LYS:N	2.42	0.49
2:B:210:ARG:HD3	2:B:264:ASP:OD2	2.12	0.49
2:D:130:ARG:O	2:D:148:ASN:HB2	2.13	0.49
2:B:364:HIS:HD2	5:C:3095:HOH:O	1.95	0.48
1:C:55:VAL:HG22	5:D:2088:HOH:O	2.12	0.48
2:B:385:ASN:C	2:B:385:ASN:HD22	2.17	0.48
2:D:149:ASN:HD22	2:D:149:ASN:N	2.09	0.48
2:D:75:3AH:HA	2:D:115:THR:O	2.12	0.48
2:D:352:GLN:HG3	5:D:2021:HOH:O	2.12	0.48
2:B:430:ARG:HB3	1:C:422:SER:HB3	1.95	0.48
2:D:116:VAL:CG2	2:D:129:PRO:HG2	2.40	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:LYS:HE2	5:C:3097:HOH:O	2.13	0.48
1:C:110:ALA:HB3	1:C:135:LYS:HB3	1.96	0.48
1:C:295:ASN:C	1:C:295:ASN:HD22	2.17	0.48
2:B:18:GLN:NE2	5:B:2021:HOH:O	2.44	0.48
2:B:83:GLY:HA3	2:B:317:VAL:O	2.13	0.48
1:A:295:ASN:ND2	1:A:297:PHE:H	2.12	0.47
1:C:36:GLY:HA2	2:D:415:GLN:O	2.14	0.47
1:A:415:GLN:O	2:B:36:GLY:HA2	2.14	0.47
2:B:75:3AH:HA	2:B:115:THR:O	2.14	0.47
1:C:14:HIS:HD2	5:C:3298:HOH:O	1.96	0.47
2:D:385:ASN:HD22	2:D:385:ASN:C	2.18	0.47
2:D:233:LYS:HB2	2:D:282:GLN:HB2	1.96	0.47
2:B:468:LYS:HD3	2:B:500:TYR:CD1	2.50	0.47
2:B:72:ARG:HG3	2:B:72:ARG:HH11	1.80	0.47
1:C:156:ARG:HH12	1:C:439:ASN:ND2	2.01	0.47
1:A:407:ASN:HD21	1:A:411:ALA:H	1.62	0.47
1:A:329:VAL:O	1:A:332:ILE:HG22	2.16	0.46
1:A:411:ALA:HB1	1:A:412:PRO:HD2	1.97	0.46
1:C:223:VAL:HG11	5:C:3374:HOH:O	2.14	0.46
1:A:119:GLU:HB2	1:C:120[B]:SER:O	2.15	0.46
2:B:339:MET:HE2	5:B:2111:HOH:O	2.14	0.46
1:C:295:ASN:HD22	1:C:296:PRO:N	2.14	0.46
1:C:411:ALA:HB1	1:C:412:PRO:HD2	1.98	0.46
2:B:295:ASN:ND2	2:B:297:PHE:H	2.14	0.46
1:C:385:ASN:C	1:C:385:ASN:HD22	2.19	0.46
1:A:91:ILE:HG21	1:A:313:VAL:HG22	1.96	0.46
1:A:394:MET:HG2	2:B:394:MET:HG2	1.97	0.46
2:B:295:ASN:HD22	2:B:296:PRO:CD	2.28	0.46
2:B:352:GLN:O	2:B:355:LEU:HB2	2.15	0.46
2:B:407:ASN:HD21	2:B:411:ALA:H	1.64	0.46
1:A:19:ARG:HD2	5:A:3355:HOH:O	2.14	0.45
2:B:143:TRP:HB2	2:B:340:PRO:HD3	1.97	0.45
1:C:388:ARG:O	2:D:67:GLU:HG2	2.17	0.45
1:A:295:ASN:HB3	1:A:298:ASP:HB2	1.98	0.45
1:A:385:ASN:HD22	1:A:387:GLN:H	1.64	0.45
2:D:275:PRO:HG2	2:D:318:LEU:HB2	1.99	0.45
1:A:407:ASN:HD22	1:A:409:PHE:N	2.02	0.45
1:C:19:ARG:NH2	1:C:24:ALA:HA	2.31	0.45
2:B:4:SER:HB2	2:B:10:ASP:OD2	2.16	0.45
1:A:468:LYS:HD3	1:A:500:TYR:HB3	1.99	0.45
1:C:109:ILE:HA	1:C:135:LYS:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:454:GLU:CD	1:C:454:GLU:H	2.19	0.44
1:A:444:ARG:HD3	1:A:485:VAL:O	2.17	0.44
2:B:149:ASN:H	2:B:149:ASN:ND2	2.13	0.44
2:B:427:GLY:N	1:C:424:GLN:HE21	2.12	0.44
1:C:75:HIS:CE1	1:C:116:VAL:HG22	2.52	0.44
1:C:446:PHE:HB2	4:C:3001:NDP:O2D	2.16	0.44
2:D:27:LEU:HD21	2:D:38:LYS:HD3	1.98	0.44
2:D:359:PRO:HG2	5:D:2084:HOH:O	2.17	0.44
1:C:93:LYS:HE3	1:C:94:TYR:CZ	2.53	0.44
1:C:129:PRO:HD3	1:C:199:LEU:HD13	1.98	0.44
2:B:144:ASP:HB2	2:B:335:ASP:O	2.17	0.44
2:B:235:HIS:NE2	2:B:282:GLN:NE2	2.65	0.44
1:A:101:GLU:HG3	1:A:102:HIS:HD2	1.83	0.44
1:A:306:LYS:HB2	5:A:3327:HOH:O	2.17	0.44
1:C:19:ARG:HH22	1:C:24:ALA:HA	1.82	0.44
1:C:233:LYS:O	1:C:281:ILE:HA	2.17	0.44
1:A:101:GLU:HG3	1:A:102:HIS:CD2	2.53	0.44
1:C:207:ASP:HA	1:C:245:LEU:HG	1.99	0.44
1:A:171:ASN:ND2	1:A:174:THR:H	2.15	0.43
1:A:369:ASN:HD21	2:B:63:HIS:CE1	2.21	0.43
2:D:206:PRO:HG3	5:D:2201:HOH:O	2.17	0.43
1:A:66:ARG:HD3	2:B:368:PRO:HG3	2.00	0.43
1:A:394:MET:HB2	2:B:394:MET:HE2	2.00	0.43
2:B:358:TYR:HB2	2:B:359:PRO:HD3	1.99	0.43
1:C:171:ASN:HB3	1:C:174:THR:OG1	2.19	0.43
2:D:203:ARG:NH2	5:D:2282:HOH:O	2.52	0.43
2:D:292:PHE:HA	2:D:293:PRO:HD3	1.85	0.43
1:A:411:ALA:HB1	1:A:412:PRO:CD	2.48	0.43
2:B:116:VAL:CG2	2:B:129:PRO:HG2	2.43	0.43
1:A:255:GLN:HG3	1:C:251:ALA:O	2.18	0.43
1:A:385:ASN:HD22	1:A:385:ASN:C	2.22	0.43
2:D:75:3AH:N2	2:D:148:ASN:CB	2.81	0.43
1:C:156:ARG:NH1	1:C:439:ASN:HD21	2.03	0.43
2:B:20:ALA:O	2:B:22:GLN:N	2.50	0.43
1:C:69:ILE:HG22	2:D:391:PRO:HG3	2.01	0.43
2:D:407:ASN:HD21	2:D:411:ALA:H	1.66	0.43
1:C:405:TYR:CD1	1:C:406:PRO:HA	2.53	0.42
1:A:391:PRO:HG3	2:B:69:ILE:HG22	2.00	0.42
2:B:171:ASN:HD22	2:B:173:GLN:N	2.16	0.42
1:A:153:PHE:CB	1:A:299:LEU:HD13	2.49	0.42
2:B:112:ARG:HD3	3:B:2001:HEM:O1D	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:VAL:O	1:C:75:HIS:HB2	2.19	0.42
1:C:444:ARG:HD3	1:C:485:VAL:O	2.18	0.42
1:A:149:ASN:HD22	1:A:149:ASN:N	2.09	0.42
2:B:233:LYS:HB2	2:B:282:GLN:HB2	2.00	0.42
1:A:178:ASP:HA	1:A:179:PRO:HD2	1.92	0.42
2:D:411:ALA:HB1	2:D:412:PRO:CD	2.50	0.42
1:A:153:PHE:HB2	1:A:299:LEU:HD13	2.02	0.42
1:A:365:ARG:HG2	1:A:366:LEU:HD13	2.01	0.42
2:B:110:ALA:HB3	2:B:135:LYS:HB3	2.02	0.42
1:A:318:LEU:HD12	1:A:318:LEU:HA	1.84	0.42
2:B:178:ASP:HA	2:B:179:PRO:HD2	1.97	0.42
2:B:214:GLY:HA3	2:B:236:TYR:CE1	2.55	0.41
1:C:499:LYS:HE3	1:C:500:TYR:HE1	1.85	0.41
1:A:395:GLN:HG3	1:A:396:ASP:N	2.28	0.41
2:D:411:ALA:HB1	2:D:412:PRO:HD2	2.03	0.41
1:C:352:GLN:HG3	5:C:3291:HOH:O	2.20	0.41
1:C:391:PRO:HG3	2:D:69:ILE:HG22	2.03	0.41
1:C:403:ASN:C	1:C:403:ASN:HD22	2.22	0.41
1:A:70:PRO:HD3	1:C:70:PRO:HG3	2.02	0.41
2:B:179:PRO:HG2	5:B:2092:HOH:O	2.21	0.41
2:D:53:GLN:NE2	5:D:2265:HOH:O	2.52	0.41
1:A:146:VAL:HB	1:A:354:ARG:HH22	1.86	0.41
2:B:385:ASN:HD22	2:B:387:GLN:H	1.69	0.41
5:B:2156:HOH:O	1:C:422:SER:HA	2.20	0.41
2:D:339:MET:HE2	5:D:2117:HOH:O	2.20	0.41
2:B:213:ASN:OD1	2:B:238:THR:HG22	2.21	0.41
2:D:334:PHE:O	2:D:362:HIS:HE1	2.04	0.41
1:A:83:GLY:HA3	1:A:317:VAL:O	2.20	0.40
2:B:75:3AH:N2	2:B:148:ASN:CB	2.80	0.40
2:D:385:ASN:HD22	2:D:387:GLN:H	1.69	0.40
1:A:255:GLN:HB2	1:C:255:GLN:HB2	2.02	0.40
1:A:295:ASN:HD22	1:A:296:PRO:CD	2.34	0.40
2:B:429:VAL:O	2:B:429:VAL:HG12	2.22	0.40
1:C:394:MET:HG2	2:D:394:MET:CG	2.43	0.40
1:A:179:PRO:HG2	5:A:3253:HOH:O	2.20	0.40
1:A:358:TYR:HB2	1:A:359:PRO:HD3	2.03	0.40
2:B:75:3AH:HN1	2:B:131:GLY:HA2	1.87	0.40
1:C:385:ASN:ND2	1:C:387:GLN:H	2.18	0.40
2:B:40:ASN:ND2	2:D:433:ASN:HA	2.37	0.40
2:B:359:PRO:O	2:B:363:ARG:HG3	2.22	0.40
1:C:33:ASN:HA	1:C:34:PRO:HD3	1.95	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:PRO:HG3	5:C:3163:HOH:O	2.22	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	497/498 (100%)	476 (96%)	19 (4%)	2 (0%)	34	30
1	C	498/498 (100%)	470 (94%)	26 (5%)	2 (0%)	34	30
2	B	497/498 (100%)	471 (95%)	24 (5%)	2 (0%)	34	30
2	D	497/498 (100%)	475 (96%)	22 (4%)	0	100	100
All	All	1989/1992 (100%)	1892 (95%)	91 (5%)	6 (0%)	41	37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	22	GLN
2	B	22	GLN
1	C	438	ASP
1	A	20	ALA
1	A	23	LYS
2	B	18	GLN

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	429/429 (100%)	413 (96%)	16 (4%)	34	32
1	C	430/429 (100%)	414 (96%)	16 (4%)	34	32
2	B	429/428 (100%)	413 (96%)	16 (4%)	34	32
2	D	429/428 (100%)	413 (96%)	16 (4%)	34	32
All	All	1717/1714 (100%)	1653 (96%)	64 (4%)	34	32

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	LYS
1	A	132	PHE
1	A	149	ASN
1	A	226	ASN
1	A	236	TYR
1	A	255	GLN
1	A	295	ASN
1	A	299	LEU
1	A	318	LEU
1	A	355	LEU
1	A	366	LEU
1	A	374	PRO
1	A	385	ASN
1	A	394	MET
1	A	489	TYR
1	A	492	HIS
2	B	5	ARG
2	B	93	LYS
2	B	132	PHE
2	B	138	THR
2	B	149	ASN
2	B	160	LEU
2	B	236	TYR
2	B	295	ASN
2	B	299	LEU
2	B	316	LEU
2	B	355	LEU
2	B	366	LEU
2	B	385	ASN
2	B	394	MET
2	B	403	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	489	TYR
1	C	5	ARG
1	C	41	VAL
1	C	93	LYS
1	C	132	PHE
1	C	149	ASN
1	C	160	LEU
1	C	188	LEU
1	C	236	TYR
1	C	255	GLN
1	C	295	ASN
1	C	318	LEU
1	C	385	ASN
1	C	403	ASN
1	C	415	GLN
1	C	426	SER
1	C	492	HIS
2	D	5	ARG
2	D	44	VAL
2	D	58	THR
2	D	93	LYS
2	D	132	PHE
2	D	149	ASN
2	D	160	LEU
2	D	236	TYR
2	D	255	GLN
2	D	295	ASN
2	D	374	PRO
2	D	380	ARG
2	D	382	ARG
2	D	385	ASN
2	D	403	ASN
2	D	489	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	HIS
1	A	149	ASN
1	A	171	ASN
1	A	282	GLN
1	A	295	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	338	ASN
1	A	369	ASN
1	A	385	ASN
1	A	398	GLN
1	A	407	ASN
1	A	421	HIS
1	A	439	ASN
1	A	449	ASN
1	A	471	GLN
1	A	475	GLN
1	A	486	HIS
1	A	501	ASN
2	B	40	ASN
2	B	63	HIS
2	B	149	ASN
2	B	171	ASN
2	B	282	GLN
2	B	295	ASN
2	B	338	ASN
2	B	364	HIS
2	B	385	ASN
2	B	397	ASN
2	B	398	GLN
2	B	403	ASN
2	B	407	ASN
2	B	421	HIS
2	B	424	GLN
2	B	439	ASN
2	B	475	GLN
2	B	486	HIS
2	B	501	ASN
1	C	13	GLN
1	C	40	ASN
1	C	53	GLN
1	C	63	HIS
1	C	149	ASN
1	C	171	ASN
1	C	211	HIS
1	C	226	ASN
1	C	282	GLN
1	C	295	ASN
1	C	338	ASN

Continued from previous page...

Mol	Chain	Res	Type
1	C	369	ASN
1	C	385	ASN
1	C	395	GLN
1	C	398	GLN
1	C	403	ASN
1	C	407	ASN
1	C	421	HIS
1	C	424	GLN
1	C	439	ASN
1	C	449	ASN
1	C	475	GLN
1	C	486	HIS
1	C	501	ASN
2	D	11	GLN
2	D	13	GLN
2	D	40	ASN
2	D	53	GLN
2	D	63	HIS
2	D	148	ASN
2	D	149	ASN
2	D	295	ASN
2	D	338	ASN
2	D	369	ASN
2	D	385	ASN
2	D	398	GLN
2	D	403	ASN
2	D	407	ASN
2	D	421	HIS
2	D	471	GLN
2	D	475	GLN
2	D	486	HIS
2	D	501	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	$\#|Z| > 2$
2	3AH	D	75	2	10,17,18	1.49	4 (40%)	2,23,25	1.50	0
2	3AH	B	75	2	10,17,18	1.50	3 (30%)	2,23,25	1.29	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
2	3AH	D	75	2	-	0/5/10/12	0/2/2/2
2	3AH	B	75	2	-	0/5/10/12	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	75	3AH	C3-N3A	2.64	1.39	1.33
2	B	75	3AH	C5-N4	-2.48	1.32	1.35
2	D	75	3AH	C3-N3A	2.41	1.38	1.33
2	D	75	3AH	C3-N4	-2.08	1.31	1.34
2	D	75	3AH	C5-N4	-2.06	1.32	1.35
2	B	75	3AH	N1-N2	-2.06	1.33	1.37
2	D	75	3AH	N1-N2	-2.02	1.33	1.37

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	75	3AH	5	0
2	B	75	3AH	4	0

5.5　Carbohydrates (i)

There are no monosaccharides in this entry.

5.6　Ligand geometry (i)

6 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	HEM	D	2003	2	41,50,50	1.20	2 (4%)	45,82,82	1.18	2 (4%)
3	HEM	B	2001	2	41,50,50	1.23	3 (7%)	45,82,82	1.23	6 (13%)
3	HEM	C	2002	1	41,50,50	1.22	1 (2%)	45,82,82	1.25	4 (8%)
3	HEM	A	2000	1	41,50,50	1.12	2 (4%)	45,82,82	1.20	3 (6%)
4	NDP	A	3000	-	45,52,52	1.35	4 (8%)	53,80,80	1.24	7 (13%)
4	NDP	C	3001	-	45,52,52	1.40	5 (11%)	53,80,80	1.30	5 (9%)

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	HEM	D	2003	2	-	4/12/54/54	-
3	HEM	B	2001	2	-	4/12/54/54	-
3	HEM	C	2002	1	-	6/12/54/54	-
3	HEM	A	2000	1	-	4/12/54/54	-
4	NDP	A	3000	-	-	3/30/77/77	0/5/5/5
4	NDP	C	3001	-	-	2/30/77/77	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3000	NDP	C4N-C3N	-4.58	1.40	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3001	NDP	C4N-C3N	-4.57	1.40	1.49
3	D	2003	HEM	C3C-C2C	-4.36	1.34	1.40
3	B	2001	HEM	C3C-C2C	-4.16	1.34	1.40
3	C	2002	HEM	C3C-C2C	-4.04	1.34	1.40
4	C	3001	NDP	C6N-C5N	3.86	1.40	1.33
4	A	3000	NDP	C6N-C5N	3.73	1.40	1.33
3	A	2000	HEM	C3C-C2C	-3.46	1.35	1.40
4	A	3000	NDP	C4N-C5N	-3.19	1.40	1.48
4	C	3001	NDP	C4N-C5N	-3.16	1.40	1.48
4	A	3000	NDP	C7N-C3N	2.77	1.54	1.48
3	A	2000	HEM	CAA-C2A	2.54	1.55	1.52
4	C	3001	NDP	C7N-C3N	2.36	1.53	1.48
3	D	2003	HEM	C3C-CAC	2.24	1.52	1.47
4	C	3001	NDP	P2B-O2B	2.22	1.63	1.59
3	B	2001	HEM	C1A-CHA	-2.05	1.35	1.41
3	B	2001	HEM	C4A-CHB	-2.04	1.35	1.41

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3001	NDP	N3A-C2A-N1A	-4.37	121.85	128.68
4	A	3000	NDP	N3A-C2A-N1A	-4.29	121.97	128.68
3	C	2002	HEM	CMA-C3A-C4A	-3.91	122.46	128.46
3	D	2003	HEM	CMA-C3A-C4A	-3.65	122.86	128.46
3	A	2000	HEM	CMA-C3A-C4A	-3.59	122.95	128.46
3	B	2001	HEM	CMA-C3A-C4A	-3.21	123.53	128.46
3	D	2003	HEM	CMA-C3A-C2A	3.16	130.90	124.94
4	A	3000	NDP	C1B-N9A-C4A	-3.07	121.24	126.64
3	C	2002	HEM	C4B-CHC-C1C	2.79	126.23	122.56
3	C	2002	HEM	CMA-C3A-C2A	2.66	129.96	124.94
3	B	2001	HEM	C4C-CHD-C1D	2.48	125.83	122.56
3	C	2002	HEM	CBA-CAA-C2A	-2.45	108.44	112.62
3	B	2001	HEM	CBA-CAA-C2A	-2.43	108.48	112.62
3	A	2000	HEM	C4C-CHD-C1D	2.40	125.73	122.56
4	C	3001	NDP	C1B-N9A-C4A	-2.40	122.42	126.64
4	A	3000	NDP	C5A-C6A-N6A	2.39	123.98	120.35
4	C	3001	NDP	C4A-C5A-N7A	2.36	111.86	109.40
3	A	2000	HEM	CMA-C3A-C2A	2.35	129.38	124.94
3	B	2001	HEM	CMC-C2C-C3C	2.31	129.00	124.68
4	C	3001	NDP	O2B-P2B-O1X	-2.25	100.70	109.39
4	C	3001	NDP	C3N-C2N-N1N	-2.22	119.93	123.10
3	B	2001	HEM	C3B-C2B-C1B	2.13	108.06	106.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2001	HEM	C4A-C3A-C2A	2.12	108.47	107.00
4	A	3000	NDP	C5A-C6A-N1A	-2.12	115.55	120.35
4	A	3000	NDP	O2B-P2B-O1X	-2.09	101.33	109.39
4	A	3000	NDP	C2A-N1A-C6A	2.04	122.25	118.75
4	A	3000	NDP	C3N-C2N-N1N	-2.04	120.18	123.10

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2002	HEM	C2B-C3B-CAB-CBB
4	A	3000	NDP	O4D-C1D-N1N-C6N
4	A	3000	NDP	O4B-C4B-C5B-O5B
4	C	3001	NDP	O4D-C1D-N1N-C6N
3	D	2003	HEM	CAD-CBD-CGD-O2D
3	D	2003	HEM	CAD-CBD-CGD-O1D
3	B	2001	HEM	CAD-CBD-CGD-O2D
3	C	2002	HEM	CAD-CBD-CGD-O2D
3	C	2002	HEM	CAA-CBA-CGA-O1A
3	A	2000	HEM	CAD-CBD-CGD-O2D
3	A	2000	HEM	CAA-CBA-CGA-O1A
3	C	2002	HEM	C4B-C3B-CAB-CBB
3	B	2001	HEM	CAD-CBD-CGD-O1D
3	C	2002	HEM	CAD-CBD-CGD-O1D
3	A	2000	HEM	CAD-CBD-CGD-O1D
3	A	2000	HEM	CAA-CBA-CGA-O2A
3	B	2001	HEM	CAA-CBA-CGA-O1A
4	A	3000	NDP	C3B-C4B-C5B-O5B
3	D	2003	HEM	CAA-CBA-CGA-O1A
3	C	2002	HEM	CAA-CBA-CGA-O2A
3	B	2001	HEM	CAA-CBA-CGA-O2A
4	C	3001	NDP	O4B-C4B-C5B-O5B
3	D	2003	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2001	HEM	1	0
4	C	3001	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 D 2003

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 2001

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM C 2002

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 2000

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP A 3000

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP C 3001

Bond lengths

Bond angles

Torsions

Rings
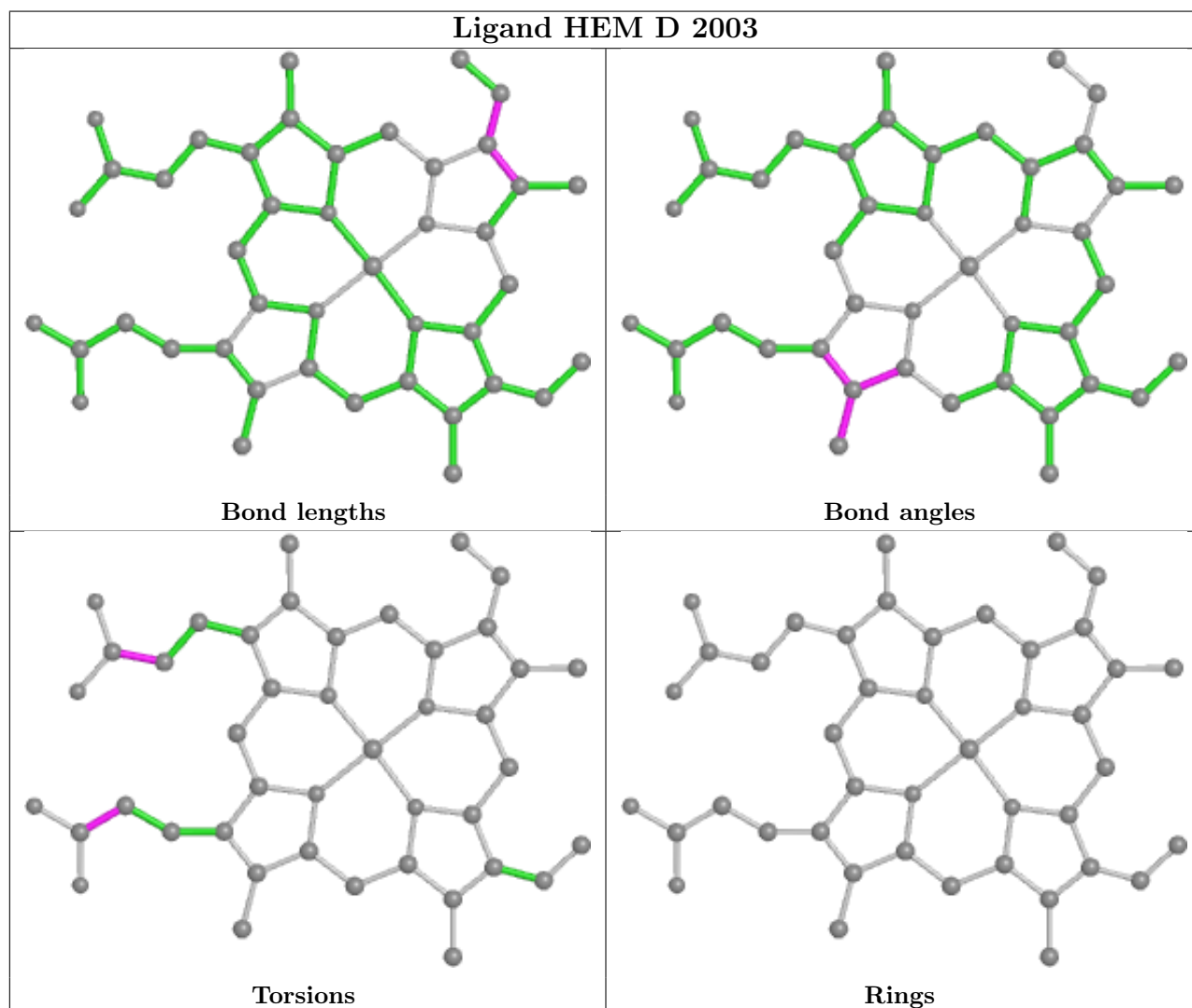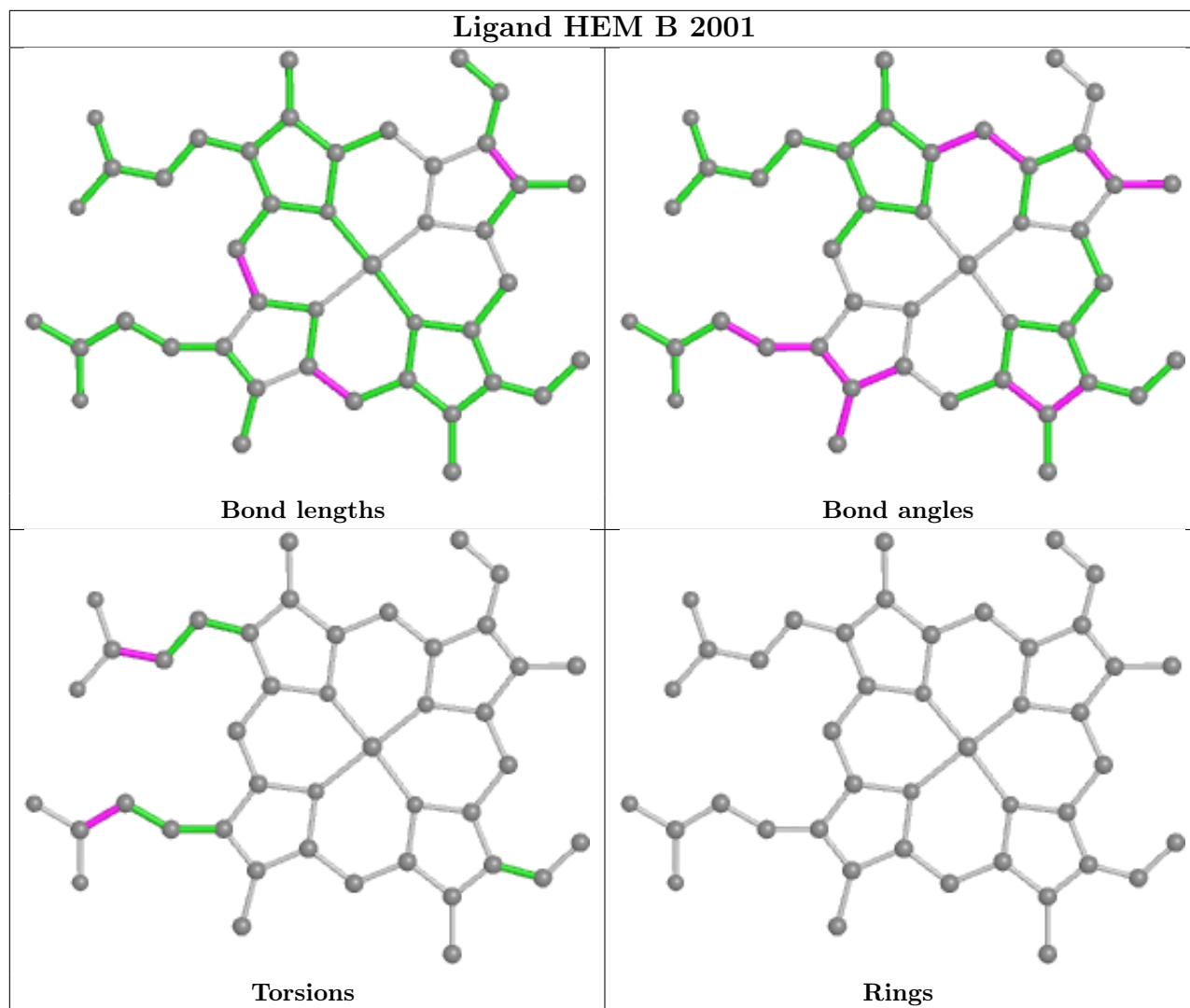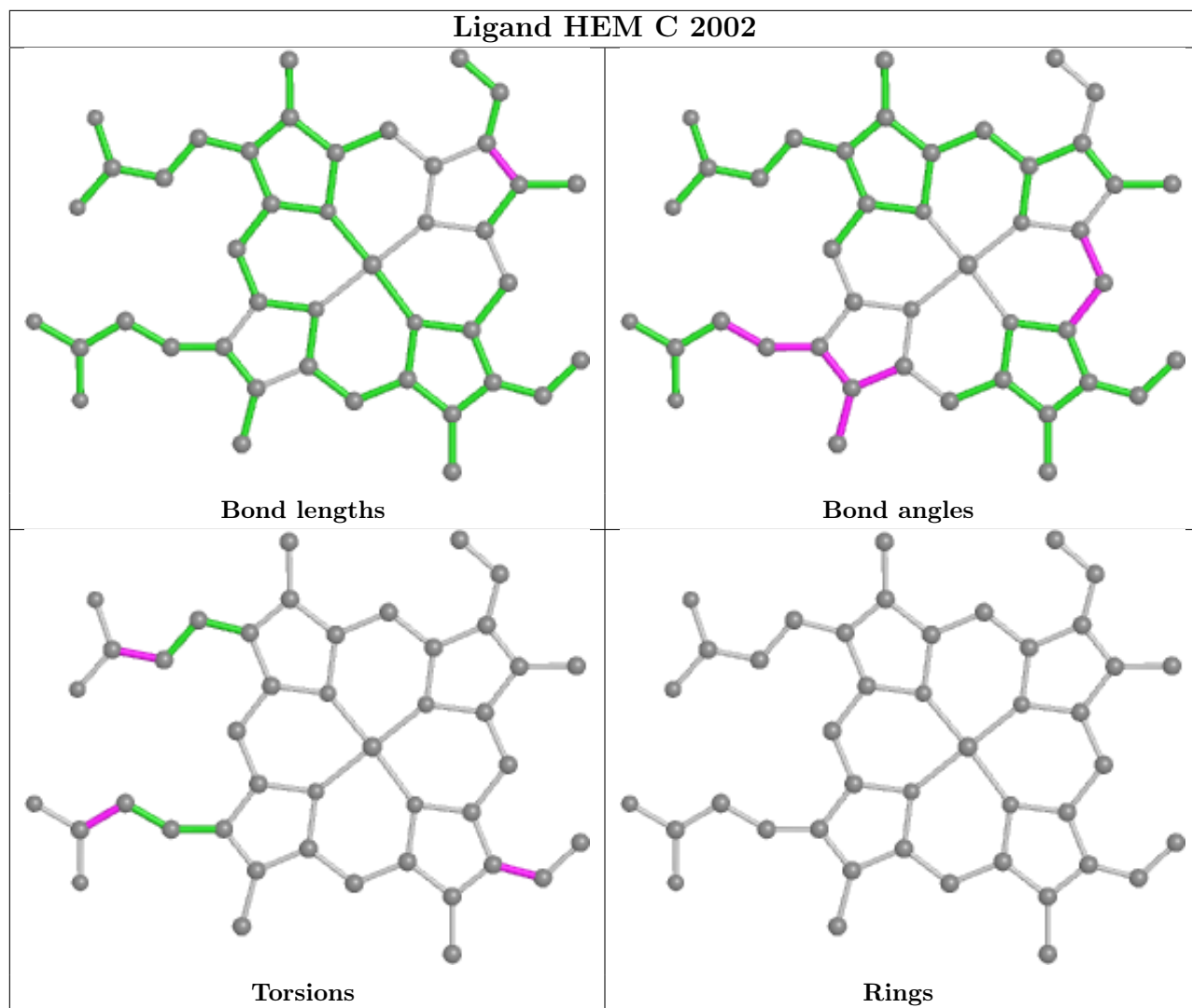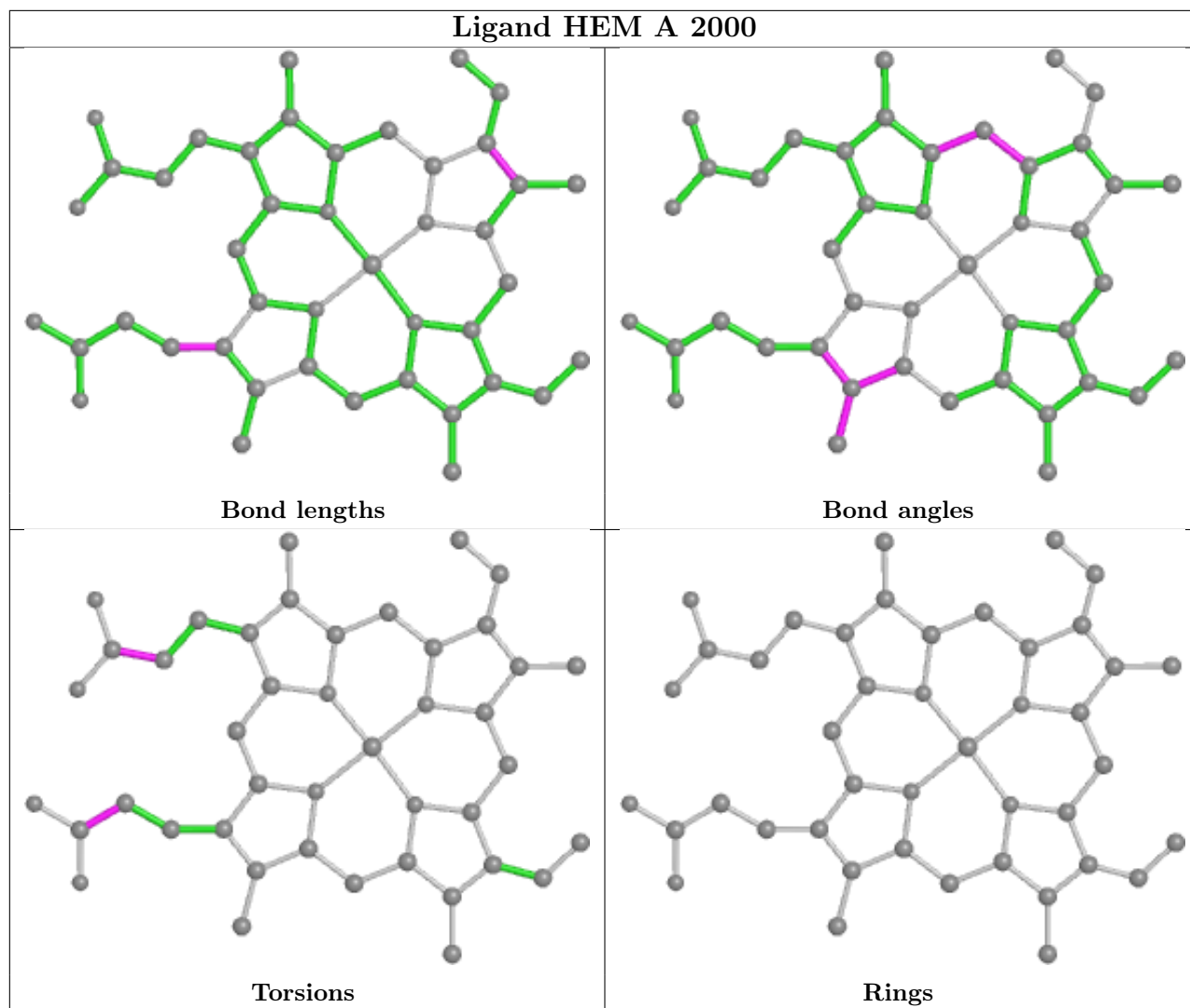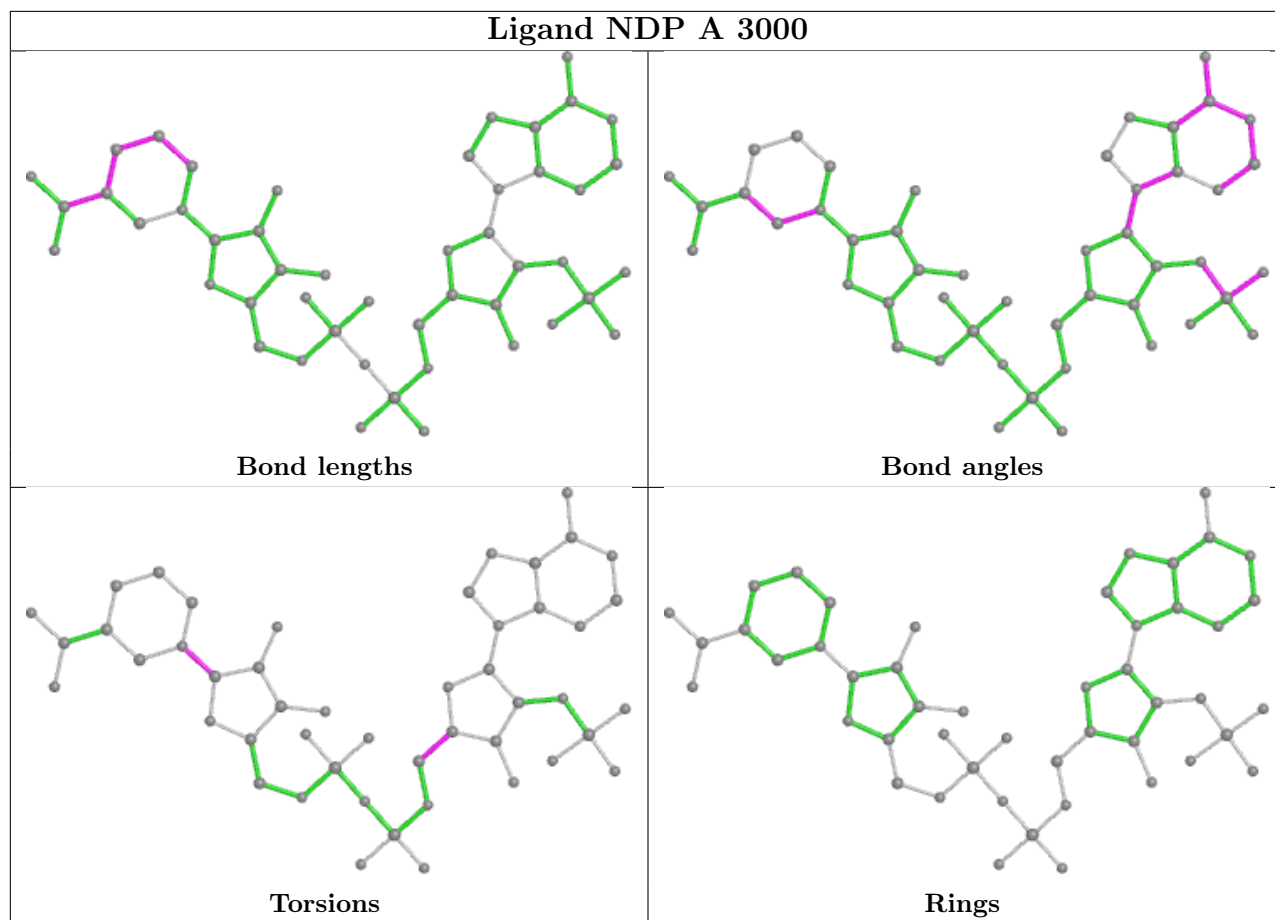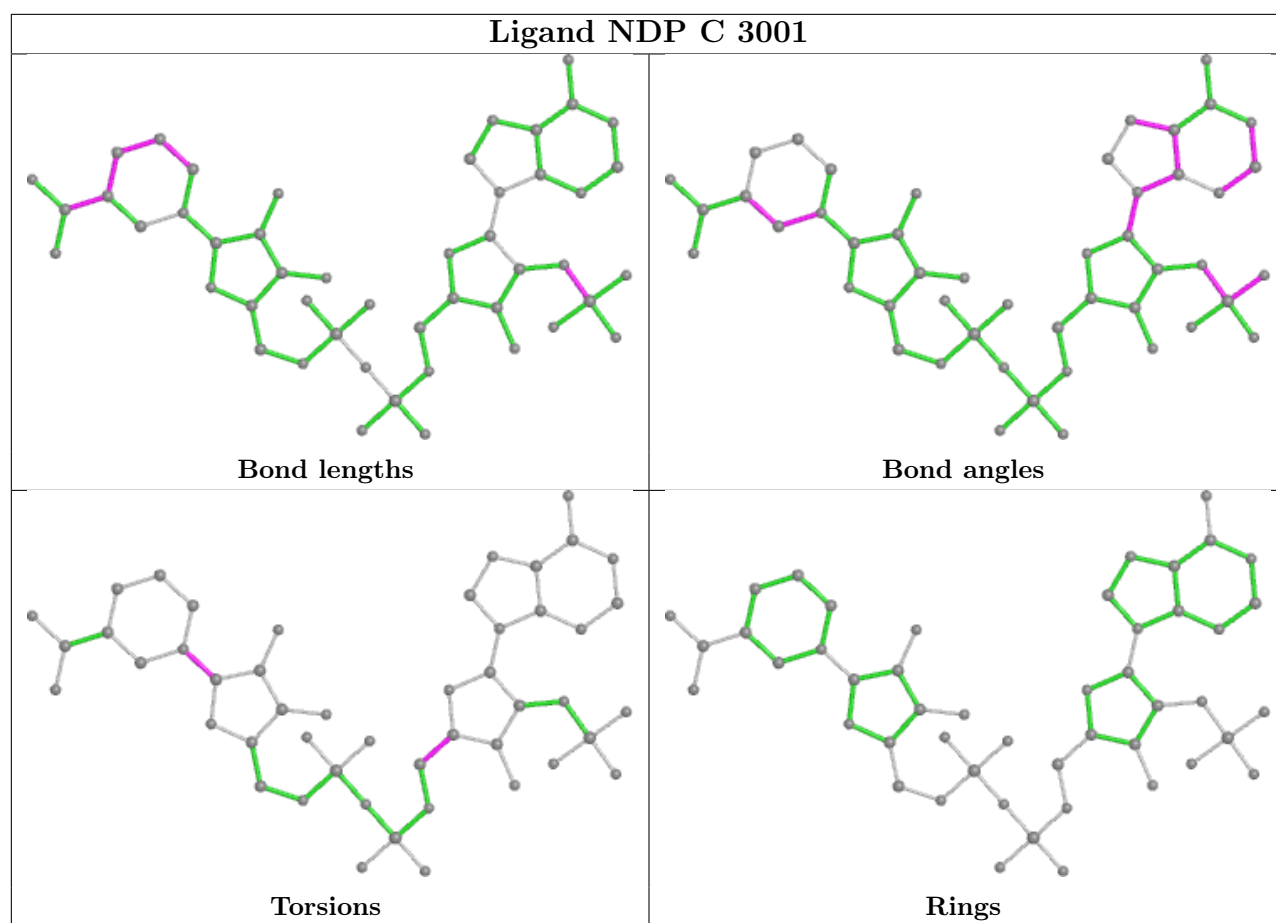
5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	497/498 (99%)	-0.34	8 (1%)	72	70	33, 38, 48, 57	0
1	C	498/498 (100%)	-0.31	11 (2%)	62	60	32, 38, 50, 60	0
2	B	497/498 (99%)	-0.26	12 (2%)	59	57	34, 39, 50, 58	0
2	D	497/498 (99%)	-0.25	12 (2%)	59	57	34, 39, 47, 58	0
All	All	1989/1992 (99%)	-0.29	43 (2%)	62	60	32, 39, 49, 60	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	21	ALA	9.1
1	C	4	SER	8.1
2	D	4	SER	7.9
1	C	22	GLN	7.2
2	B	4	SER	7.1
2	B	22	GLN	6.9
2	B	21	ALA	5.6
1	A	20	ALA	4.8
1	A	21	ALA	4.8
2	B	20	ALA	4.4
1	C	20	ALA	4.1
2	B	426	SER	3.9
2	D	20	ALA	3.7
1	C	21	ALA	3.6
2	B	306	LYS	3.2
1	C	306	LYS	2.9
2	D	382	ARG	2.9
1	A	22	GLN	2.8
2	D	248	GLU	2.8
2	D	306	LYS	2.8
2	D	22	GLN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	287	ASN	2.7
1	A	382	ARG	2.6
2	B	500	TYR	2.6
1	A	395	GLN	2.5
2	B	424	GLN	2.5
1	C	500	TYR	2.4
1	A	500	TYR	2.4
1	C	426	SER	2.3
2	B	290	GLU	2.3
1	C	415	GLN	2.3
2	D	18	GLN	2.2
1	A	488	ASP	2.2
1	A	291	THR	2.2
2	D	5	ARG	2.2
2	B	18	GLN	2.1
2	B	382	ARG	2.1
2	D	499	LYS	2.1
2	D	500	TYR	2.1
2	B	5	ARG	2.1
1	C	18	GLN	2.1
2	D	198	PHE	2.1
1	C	5	ARG	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
2	3AH	B	75	16/17	0.87	0.15	35,39,51,52	0
2	3AH	D	75	16/17	0.87	0.16	35,39,50,51	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NDP	C	3001	48/48	0.91	0.14	55,59,63,63	0
4	NDP	A	3000	48/48	0.93	0.11	48,51,57,57	0
3	HEM	A	2000	43/43	0.97	0.09	33,33,34,34	0
3	HEM	C	2002	43/43	0.97	0.10	33,34,35,35	0
3	HEM	B	2001	43/43	0.98	0.09	33,34,35,35	0
3	HEM	D	2003	43/43	0.98	0.09	33,34,35,35	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 3001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)
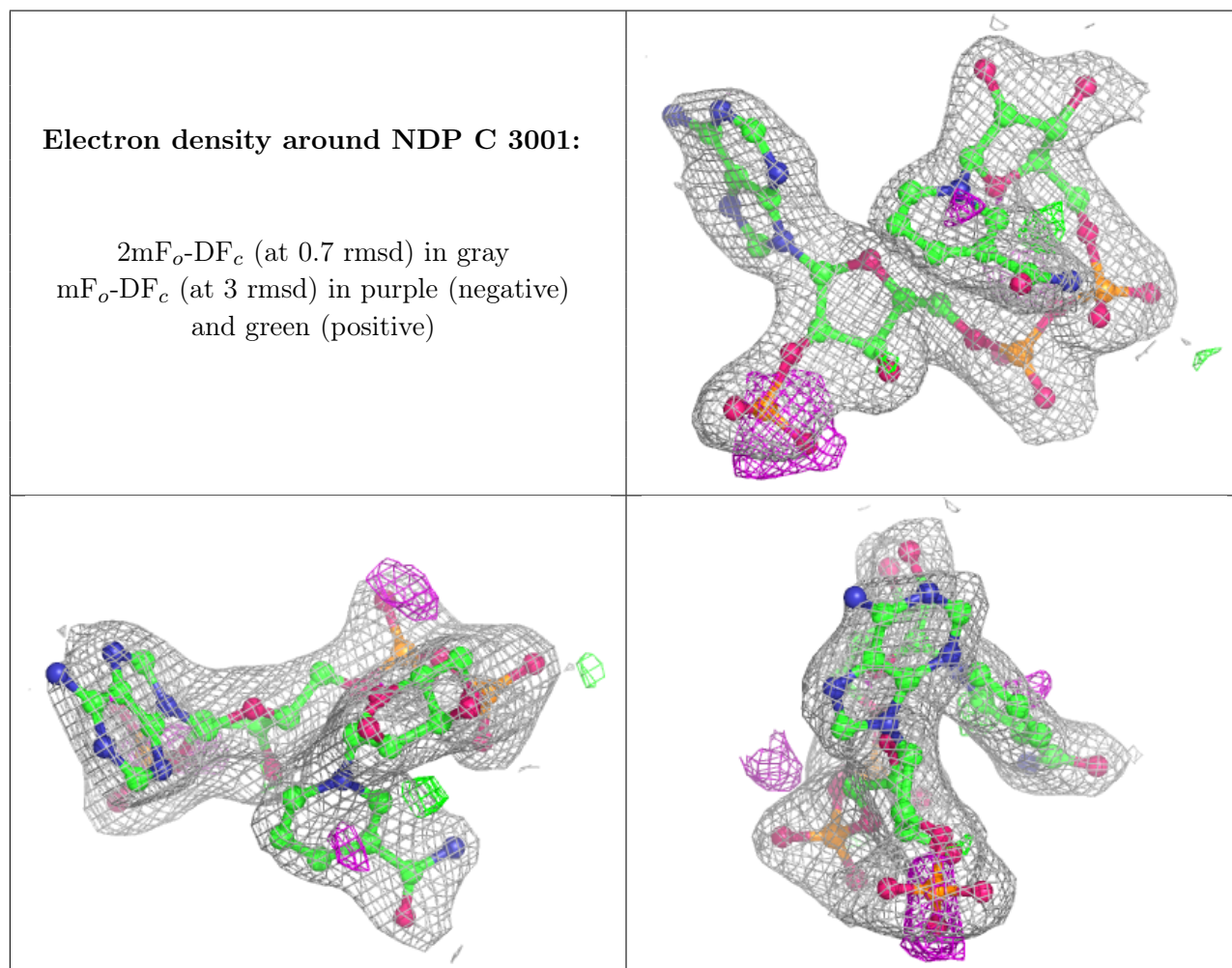
Electron density around NDP A 3000:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
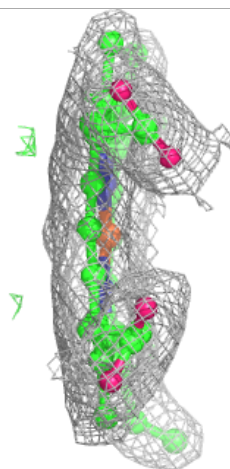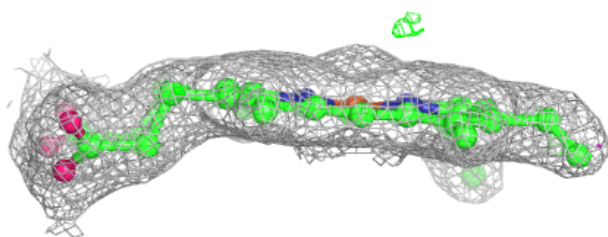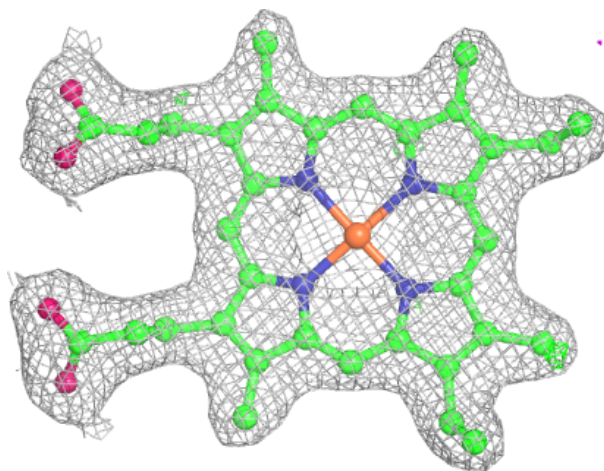$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
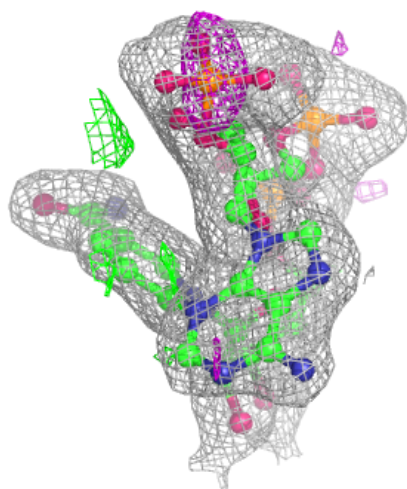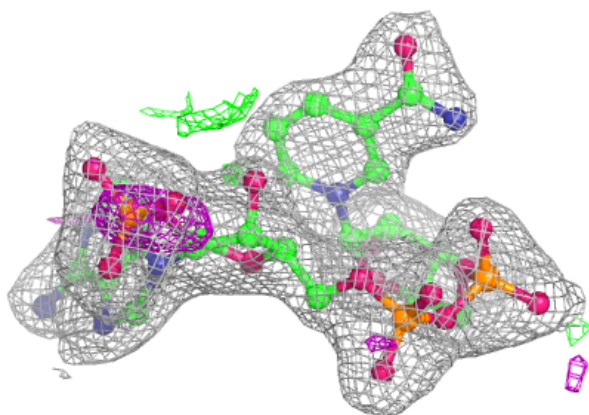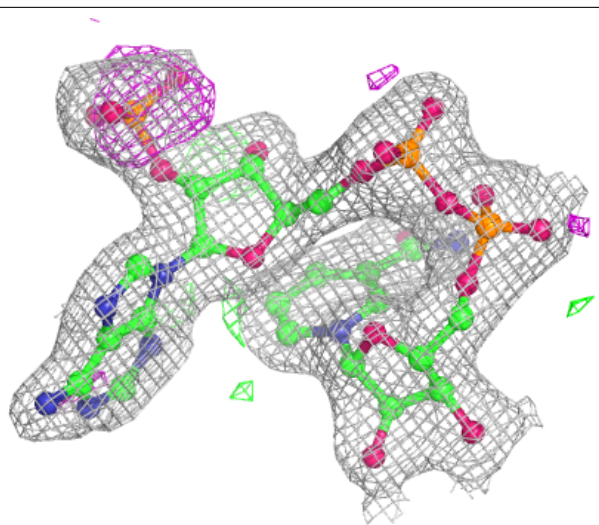
Electron density around HEM A 2000:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
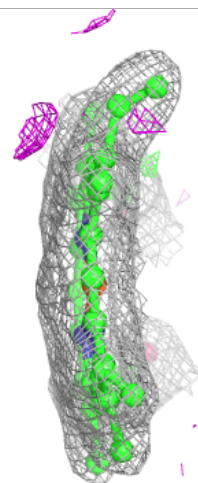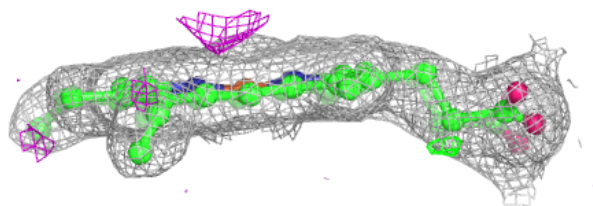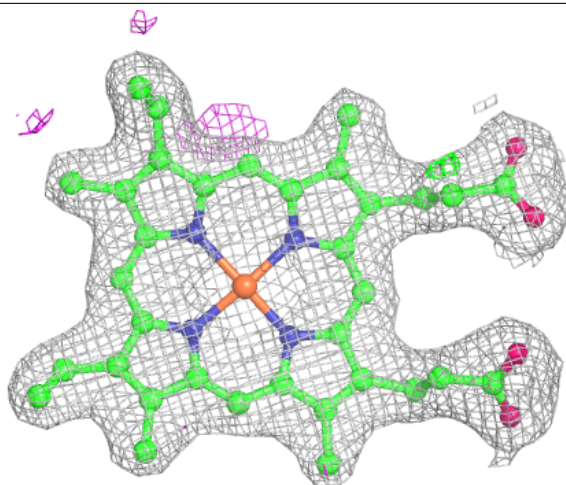mF_o-DF_c (at 3 rmsd) in purple (negative)
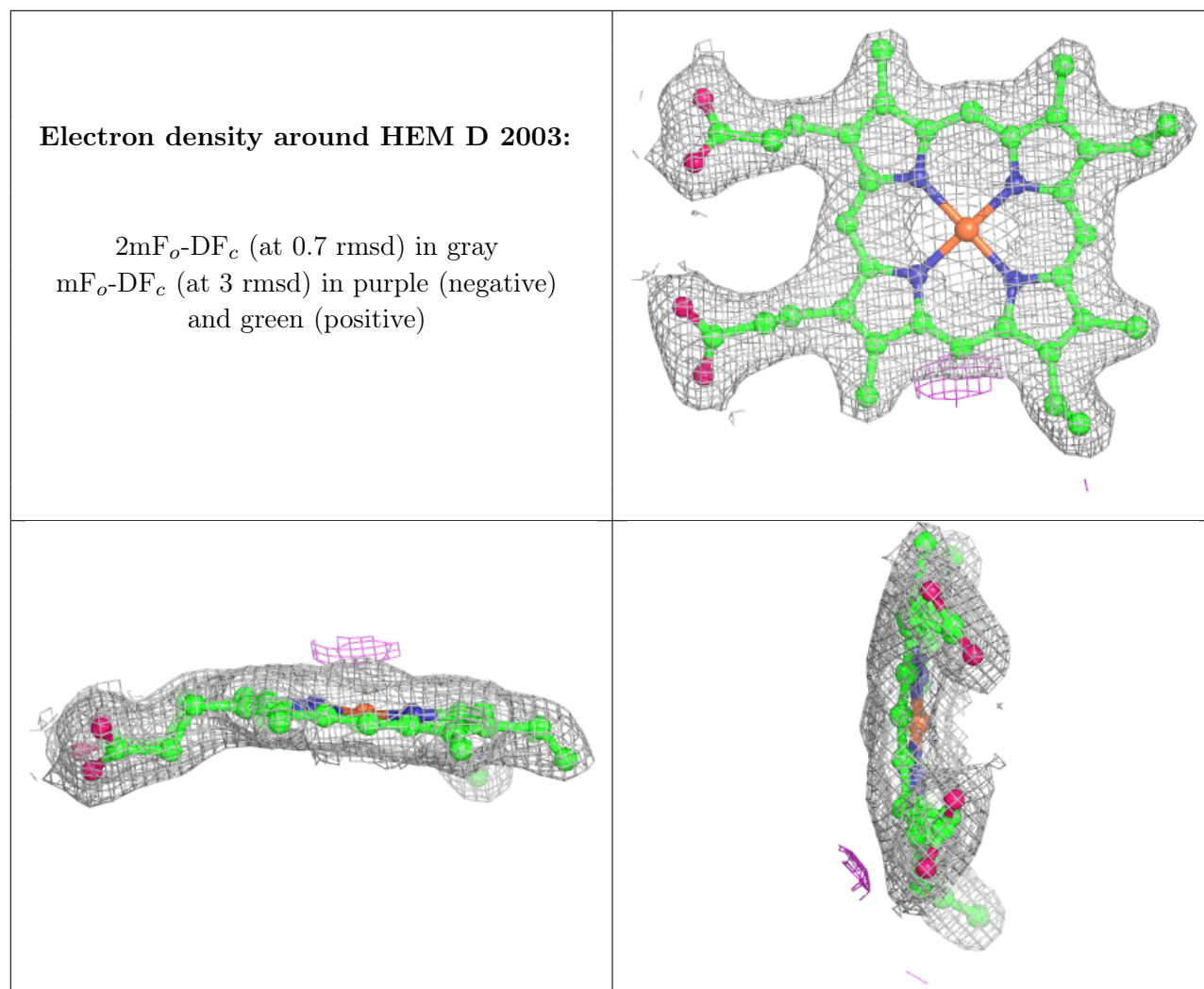and green (positive)
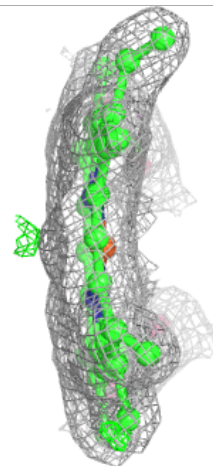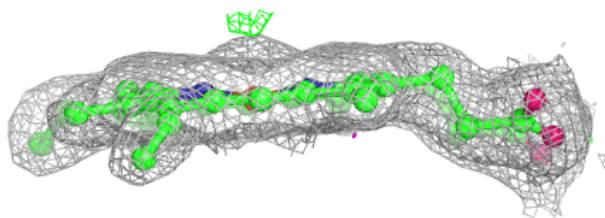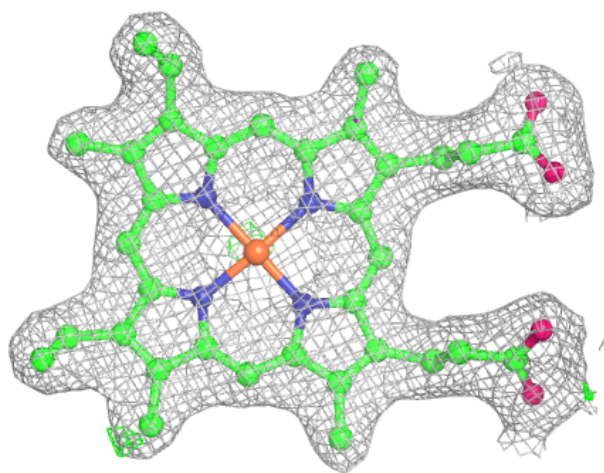
Electron density around HEM C 2002:

$2mF_o$-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 2001:

$2mF_o$-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 D 2003:

$2mF_o$-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.