



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2023 – 12:29 PM EDT

PDB ID : 1DGF  
Title : HUMAN ERYTHROCYTE CATALASE  
Authors : Putnam, C.D.; Arvai, A.S.; Bourne, Y.; Tainer, J.A.  
Deposited on : 1999-11-24  
Resolution : 1.50 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](mailto: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>.

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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 : 2.35.1  
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

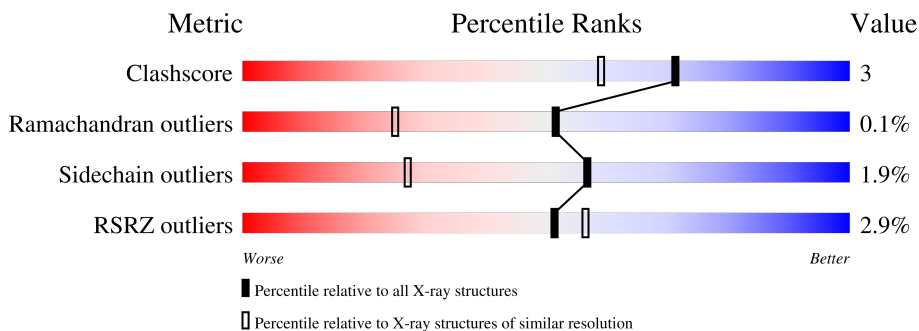
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	497	
1	B	497	
1	C	497	
1	D	497	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	A	5000	-	X	-	-
2	ACT	B	5002	-	X	X	-
2	ACT	C	5001	-	X	-	-
2	ACT	D	5003	-	X	-	-

## 2 Entry composition [i](#)

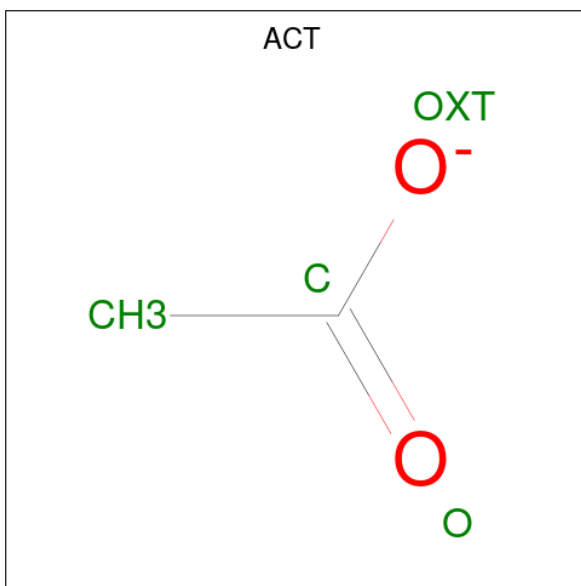
There are 5 unique types of molecules in this entry. The entry contains 18675 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	497	4028	2557	716	741	14	0	4	0
1	B	497	4028	2557	716	741	14	0	4	0
1	C	497	4018	2551	713	740	14	0	3	0
1	D	497	4018	2551	713	740	14	0	3	0

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



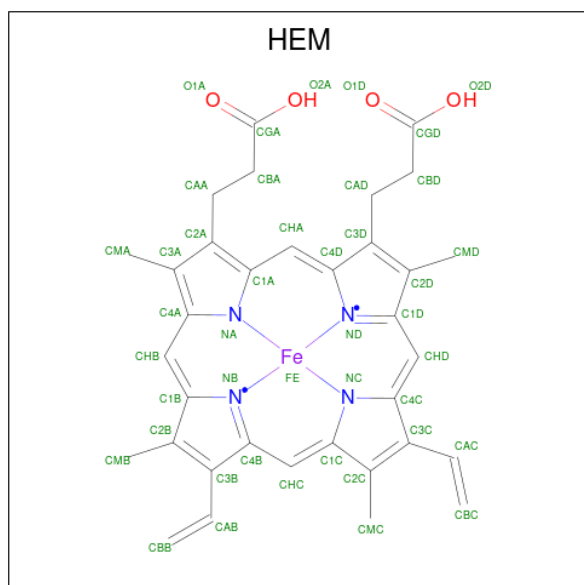
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	4	2	2	0	0
2	B	1	4	2	2	0	0

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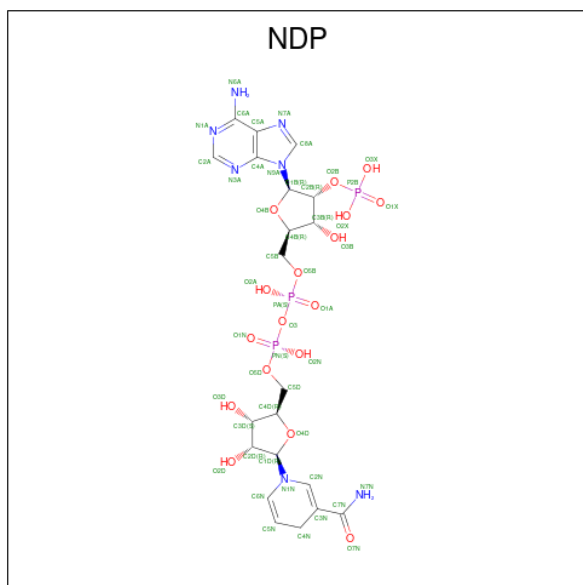
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

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

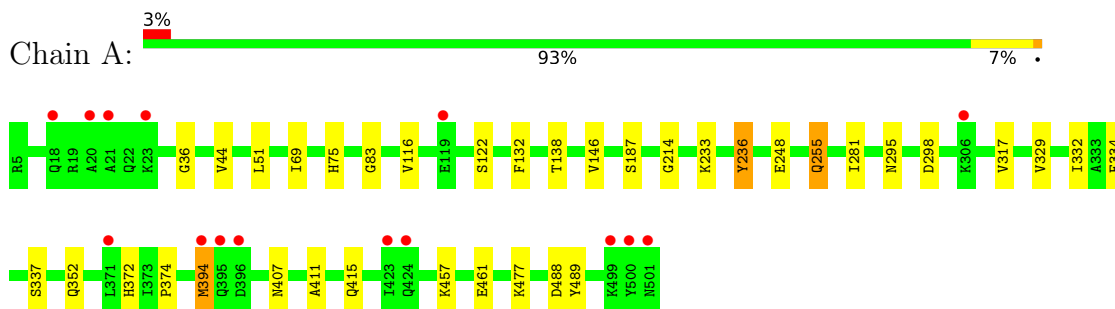
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	564	Total	O	0	0
			564	564		
5	B	590	Total	O	0	0
			590	590		
5	C	570	Total	O	0	0
			570	570		
5	D	575	Total	O	0	0
			575	575		

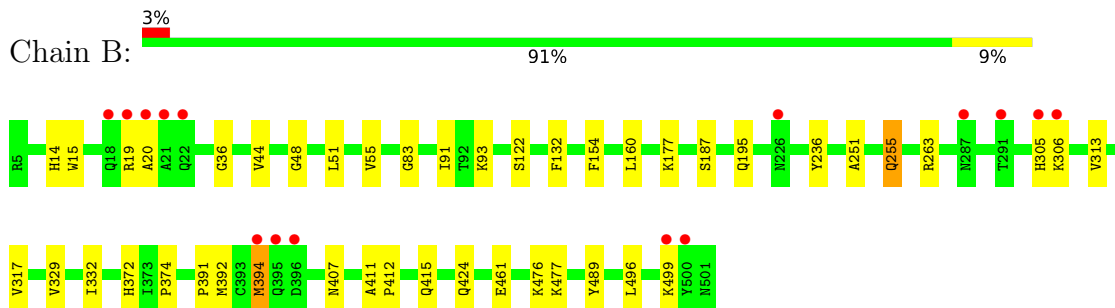
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

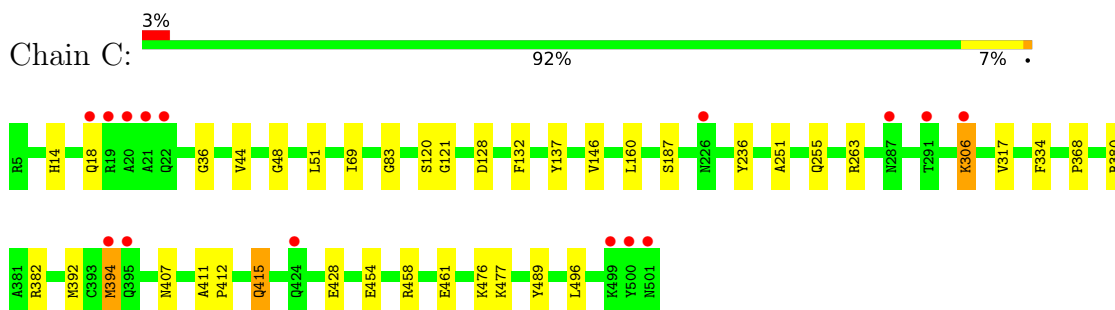
- Molecule 1: CATALASE



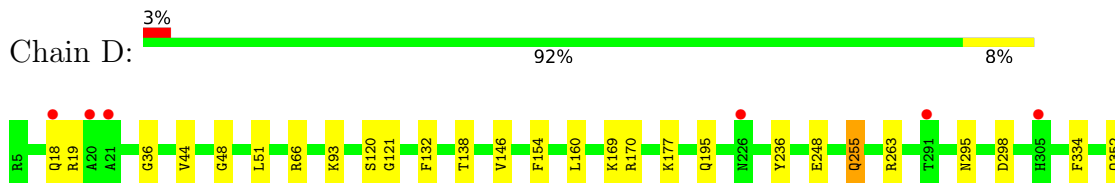
- Molecule 1: CATALASE

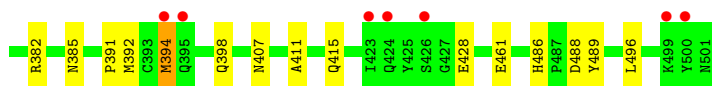


- Molecule 1: CATALASE



- Molecule 1: CATALASE







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.72Å 142.50Å 232.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.50 19.96 – 1.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.50) 90.9 (19.96-1.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 1.50Å)	Xtrriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.172 , 0.192 0.165 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.1	Xtrriage
Anisotropy	0.017	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 56.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	18675	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, 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	0.36	0/4148	0.62	1/5635 (0.0%)
1	B	0.35	0/4148	0.62	0/5635
1	C	0.35	0/4137	0.62	0/5620
1	D	0.35	0/4137	0.62	0/5620
All	All	0.35	0/16570	0.62	1/22510 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	MET	N-CA-C	5.14	124.88	111.00

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	4028	0	3851	26	0
1	B	4028	0	3851	37	0
1	C	4018	0	3845	31	0
1	D	4018	0	3845	34	0
2	A	4	0	3	0	0
2	B	4	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	4	0	3	1	0
2	D	4	0	0	1	0
3	A	43	0	30	0	0
3	B	43	0	30	0	0
3	C	43	0	30	0	0
3	D	43	0	30	0	0
4	A	48	0	26	0	0
4	C	48	0	26	0	0
5	A	564	0	0	4	0
5	B	590	0	0	7	0
5	C	570	0	0	4	0
5	D	575	0	0	8	0
All	All	18675	0	15570	111	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 (111) 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:B:5002:ACT:OXT	2:B:5002:ACT:C	1.64	1.45
2:C:5001:ACT:OXT	2:C:5001:ACT:C	1.65	1.41
2:D:5003:ACT:O	2:D:5003:ACT:C	1.78	1.29
1:B:306:LYS:HD2	1:B:306:LYS:H	1.27	0.96
1:D:385:ASN:H	1:D:398:GLN:HE22	1.27	0.82
1:B:476:LYS:HA	1:B:476:LYS:HZ2	1.45	0.81
1:D:486:HIS:HD2	1:D:488:ASP:H	1.29	0.80
1:C:306:LYS:HZ2	1:C:306:LYS:H	1.35	0.72
1:D:19:ARG:HH11	1:D:19:ARG:HG3	1.53	0.72
1:D:120[B]:SER:O	5:D:5194:HOH:O	2.09	0.71
1:A:394:MET:SD	1:B:374:PRO:HD3	2.32	0.69
1:A:372[B]:HIS:HD2	1:A:394:MET:H	1.39	0.68
1:B:15:TRP:CH2	1:B:19:ARG:HD2	2.30	0.66
1:C:382:ARG:HG2	1:C:382:ARG:HH21	1.64	0.62
1:D:392:MET:HE1	1:D:394:MET:HE3	1.83	0.60
1:C:306:LYS:HB2	1:C:306:LYS:HZ3	1.68	0.58
1:D:486:HIS:CD2	1:D:488:ASP:H	2.16	0.58
1:A:372[B]:HIS:CD2	1:A:394:MET:H	2.21	0.58
1:B:122:SER:HA	1:D:121[B]:GLY:O	2.04	0.58
1:B:306:LYS:H	1:B:306:LYS:CD	2.05	0.57
1:B:372[B]:HIS:HD2	1:B:394:MET:H	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372[B]:HIS:HB3	1:B:394:MET:HE2	1.87	0.57
1:B:305:HIS:HB3	5:B:5140:HOH:O	2.06	0.56
1:C:120[B]:SER:O	5:C:5248:HOH:O	2.17	0.56
1:C:454:GLU:HG2	1:C:458:ARG:HH12	1.70	0.56
1:C:306:LYS:H	1:C:306:LYS:NZ	2.03	0.55
1:C:476:LYS:HD2	5:C:5162:HOH:O	2.07	0.55
1:A:407:ASN:HD21	1:A:411:ALA:HB3	1.72	0.55
1:C:415:GLN:O	1:D:36:GLY:HA2	2.08	0.54
1:B:255:GLN:HB2	1:D:255:GLN:HB2	1.90	0.53
1:A:122:SER:HA	1:C:121[B]:GLY:O	2.09	0.53
1:B:305:HIS:CE1	1:B:306:LYS:HE3	2.44	0.53
1:C:407:ASN:HD21	1:C:411:ALA:HB3	1.72	0.53
1:C:392:MET:HE2	5:D:5058:HOH:O	2.10	0.52
1:B:306:LYS:HD2	1:B:306:LYS:N	2.10	0.51
1:D:407:ASN:HD21	1:D:411:ALA:HB3	1.76	0.51
1:A:36:GLY:HA2	1:B:415:GLN:O	2.11	0.51
1:C:44:VAL:O	1:C:48:GLY:HA3	2.11	0.51
1:B:187:SER:HB2	1:B:477:LYS:HG2	1.91	0.50
1:B:44:VAL:O	1:B:48:GLY:HA3	2.11	0.49
1:C:187:SER:HB2	1:C:477:LYS:HG2	1.94	0.49
1:B:19:ARG:HD3	5:B:5130:HOH:O	2.13	0.49
1:D:19:ARG:NH1	5:D:5254:HOH:O	2.46	0.49
1:C:454:GLU:HG2	1:C:458:ARG:NH1	2.26	0.48
1:A:51:LEU:HD13	1:D:51:LEU:HD13	1.95	0.48
1:B:14:HIS:HD2	5:B:5269:HOH:O	1.95	0.48
1:B:407:ASN:HD21	1:B:411:ALA:HB3	1.79	0.48
1:A:415:GLN:O	1:B:36:GLY:HA2	2.12	0.47
1:A:69:ILE:HG22	1:B:391:PRO:HG3	1.96	0.47
2:B:5002:ACT:C	5:B:5479:HOH:O	2.63	0.47
1:C:382:ARG:HG2	1:C:382:ARG:NH2	2.28	0.47
1:A:394:MET:HG3	1:B:394:MET:HG2	1.97	0.47
1:D:44:VAL:O	1:D:48:GLY:HA3	2.14	0.47
2:B:5002:ACT:OXT	2:B:5002:ACT:CH3	2.44	0.47
1:B:91:ILE:HG21	1:B:313:VAL:HG22	1.97	0.46
1:A:146:VAL:HG22	1:A:334:PHE:HB3	1.99	0.45
1:A:295:ASN:HB3	1:A:298:ASP:HB2	1.99	0.45
5:A:5061:HOH:O	1:B:392:MET:HE2	2.17	0.45
1:C:394:MET:HG2	1:D:394:MET:HG2	1.99	0.45
1:C:461:GLU:HA	1:C:496:LEU:HD13	1.98	0.45
1:B:263:ARG:HD3	5:B:5412:HOH:O	2.16	0.45
1:C:146:VAL:HG22	1:C:334:PHE:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:MET:HB2	1:D:394:MET:HE2	1.98	0.45
1:A:44:VAL:HG21	1:D:44:VAL:HG11	1.98	0.45
1:A:352:GLN:HG3	5:A:5265:HOH:O	2.17	0.44
1:B:251:ALA:O	1:D:255:GLN:HG3	2.17	0.44
1:A:187:SER:HB2	1:A:477:LYS:HG3	1.99	0.44
1:D:263:ARG:HD3	5:D:5411:HOH:O	2.17	0.44
1:B:55:VAL:HG12	5:B:5572:HOH:O	2.16	0.44
1:A:83:GLY:HA3	1:A:317:VAL:O	2.18	0.44
1:D:177:LYS:HA	1:D:177:LYS:HE2	1.98	0.44
1:D:169:LYS:HB3	5:D:5234:HOH:O	2.18	0.44
1:B:51:LEU:HD13	1:C:51:LEU:HD13	2.00	0.43
1:B:411:ALA:HB1	1:B:412:PRO:HD2	2.01	0.43
1:C:368:PRO:HG3	1:D:66:ARG:HD3	2.01	0.43
1:D:19:ARG:HH11	1:D:19:ARG:CG	2.27	0.43
1:B:424:GLN:HA	1:C:428:GLU:HA	2.01	0.43
1:A:457:LYS:O	1:A:461:GLU:HG3	2.18	0.43
1:C:411:ALA:HB1	1:C:412:PRO:HD2	2.00	0.43
1:D:295:ASN:HB3	1:D:298:ASP:HB2	2.01	0.43
1:C:36:GLY:HA2	1:D:415:GLN:O	2.19	0.42
1:D:146:VAL:HG22	1:D:334:PHE:HB3	2.01	0.42
1:B:154:PHE:CE2	1:B:195:GLN:HG3	2.55	0.42
1:A:488:ASP:HB3	5:A:5482:HOH:O	2.20	0.42
1:C:137:TYR:O	1:C:380:ARG:HD3	2.19	0.42
1:B:499:LYS:HE2	1:B:499:LYS:HB3	1.89	0.42
1:A:248:GLU:HB2	5:A:5356:HOH:O	2.19	0.42
1:B:411:ALA:HB1	1:B:412:PRO:CD	2.50	0.42
1:C:263:ARG:HD3	5:C:5491:HOH:O	2.18	0.42
1:D:248:GLU:H	1:D:248:GLU:CD	2.23	0.42
1:B:329:VAL:O	1:B:332:ILE:HG22	2.20	0.42
1:C:411:ALA:HB1	1:C:412:PRO:CD	2.50	0.42
1:B:177:LYS:NZ	5:B:5537:HOH:O	2.53	0.41
1:A:214:GLY:HA3	1:A:236:TYR:CE1	2.55	0.41
1:A:255:GLN:HG3	1:C:251:ALA:O	2.20	0.41
1:D:428:GLU:HG3	5:D:5324:HOH:O	2.20	0.41
1:D:352:GLN:HG3	5:D:5195:HOH:O	2.20	0.41
1:C:83:GLY:HA3	1:C:317:VAL:O	2.21	0.41
1:D:154:PHE:CE2	1:D:195:GLN:HG3	2.56	0.41
1:D:177:LYS:NZ	5:D:5224:HOH:O	2.52	0.41
1:A:75:HIS:CE1	1:A:116:VAL:HG22	2.56	0.41
1:A:329:VAL:O	1:A:332:ILE:HG22	2.21	0.41
1:B:83:GLY:HA3	1:B:317:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:ILE:HG22	1:D:391:PRO:HG3	2.03	0.41
1:A:337:SER:HB2	1:B:55:VAL:HG21	2.03	0.40
1:C:14:HIS:O	1:C:18:GLN:HG3	2.21	0.40
5:C:5073:HOH:O	1:D:392:MET:HE2	2.20	0.40
1:A:233:LYS:O	1:A:281:ILE:HA	2.21	0.40
1:D:169:LYS:HB3	1:D:170:ARG:H	1.78	0.40
1:D:461:GLU:HA	1:D:496:LEU:HD13	2.04	0.40
1:B:461:GLU:HA	1:B:496:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	499/497 (100%)	479 (96%)	20 (4%)	0	100	100
1	B	499/497 (100%)	482 (97%)	16 (3%)	1 (0%)	47	23
1	C	498/497 (100%)	479 (96%)	19 (4%)	0	100	100
1	D	498/497 (100%)	485 (97%)	13 (3%)	0	100	100
All	All	1994/1988 (100%)	1925 (96%)	68 (3%)	1 (0%)	51	25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	20	ALA

### 5.3.2 Protein sidechains [i](#)

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	431/428 (101%)	425 (99%)	6 (1%)	67	42
1	B	431/428 (101%)	424 (98%)	7 (2%)	62	36
1	C	430/428 (100%)	421 (98%)	9 (2%)	53	23
1	D	430/428 (100%)	420 (98%)	10 (2%)	50	20
All	All	1722/1712 (101%)	1690 (98%)	32 (2%)	57	27

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	PHE
1	A	138	THR
1	A	236	TYR
1	A	255	GLN
1	A	374	PRO
1	A	489	TYR
1	B	93	LYS
1	B	132	PHE
1	B	160	LEU
1	B	236	TYR
1	B	255	GLN
1	B	394	MET
1	B	489	TYR
1	C	128	ASP
1	C	132	PHE
1	C	160	LEU
1	C	236	TYR
1	C	255	GLN
1	C	306	LYS
1	C	394	MET
1	C	415	GLN
1	C	489	TYR
1	D	18	GLN
1	D	93	LYS
1	D	132	PHE
1	D	138	THR
1	D	160	LEU
1	D	236	TYR
1	D	255	GLN
1	D	382	ARG

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Mol	Chain	Res	Type
1	D	394	MET
1	D	489	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	395	GLN
1	A	475	GLN
1	A	501	ASN
1	B	14	HIS
1	B	168	GLN
1	B	424	GLN
1	B	475	GLN
1	B	501	ASN
1	C	211	HIS
1	C	226	ASN
1	C	415	GLN
1	C	475	GLN
1	C	501	ASN
1	D	18	GLN
1	D	211	HIS
1	D	395	GLN
1	D	398	GLN
1	D	475	GLN
1	D	486	HIS
1	D	501	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 5.6 Ligand geometry

10 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	B	3001	1	41,50,50	1.30	5 (12%)	45,82,82	1.09	4 (8%)
4	NDP	C	4001	-	45,52,52	1.38	6 (13%)	53,80,80	1.25	6 (11%)
4	NDP	A	4000	-	45,52,52	1.44	6 (13%)	53,80,80	1.21	6 (11%)
2	ACT	C	5001	-	3,3,3	4.43	2 (66%)	3,3,3	3.15	3 (100%)
2	ACT	A	5000	-	3,3,3	5.89	3 (100%)	3,3,3	5.09	3 (100%)
3	HEM	C	3002	1	41,50,50	1.33	5 (12%)	45,82,82	1.09	3 (6%)
3	HEM	D	3003	1	41,50,50	1.27	5 (12%)	45,82,82	1.16	5 (11%)
3	HEM	A	3000	1	41,50,50	1.25	5 (12%)	45,82,82	1.20	5 (11%)
2	ACT	D	5003	-	3,3,3	8.17	3 (100%)	3,3,3	5.62	2 (66%)
2	ACT	B	5002	-	3,3,3	5.63	3 (100%)	3,3,3	1.90	1 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	B	3001	1	-	3/12/54/54	-
4	NDP	C	4001	-	-	3/30/77/77	0/5/5/5
4	NDP	A	4000	-	-	3/30/77/77	0/5/5/5
3	HEM	C	3002	1	-	3/12/54/54	-
3	HEM	D	3003	1	-	3/12/54/54	-
3	HEM	A	3000	1	-	4/12/54/54	-

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	5003	ACT	O-C	12.27	1.78	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	5001	ACT	OXT-C	7.26	1.65	1.30
2	A	5000	ACT	O-C	7.11	1.54	1.22
2	B	5002	ACT	OXT-C	7.09	1.64	1.30
2	D	5003	ACT	CH3-C	-6.46	1.22	1.49
2	B	5002	ACT	CH3-C	-6.06	1.23	1.49
2	A	5000	ACT	OXT-C	5.44	1.56	1.30
2	A	5000	ACT	CH3-C	-4.91	1.28	1.49
4	A	4000	NDP	C4N-C3N	-4.60	1.40	1.49
4	C	4001	NDP	C4N-C3N	-4.56	1.41	1.49
3	B	3001	HEM	C3C-CAC	-4.09	1.39	1.47
3	D	3003	HEM	C3C-CAC	-3.88	1.39	1.47
3	C	3002	HEM	C3C-CAC	-3.78	1.40	1.47
4	A	4000	NDP	C6N-C5N	3.75	1.40	1.33
4	C	4001	NDP	C6N-C5N	3.67	1.39	1.33
4	A	4000	NDP	C4N-C5N	-3.22	1.40	1.48
3	A	3000	HEM	C3C-CAC	-3.18	1.41	1.47
4	C	4001	NDP	C4N-C5N	-3.09	1.40	1.48
3	C	3002	HEM	CBB-CAB	2.95	1.44	1.30
4	A	4000	NDP	P2B-O2B	2.84	1.64	1.59
2	D	5003	ACT	OXT-C	2.83	1.44	1.30
2	B	5002	ACT	O-C	2.82	1.35	1.22
3	B	3001	HEM	CAB-C3B	-2.76	1.39	1.47
3	C	3002	HEM	CAB-C3B	-2.70	1.40	1.47
3	D	3003	HEM	CBB-CAB	2.70	1.43	1.30
3	B	3001	HEM	CBB-CAB	2.68	1.43	1.30
3	C	3002	HEM	C3C-C2C	-2.65	1.36	1.40
3	A	3000	HEM	CBB-CAB	2.59	1.43	1.30
3	A	3000	HEM	C3C-C2C	-2.57	1.36	1.40
3	A	3000	HEM	CAB-C3B	-2.47	1.40	1.47
3	B	3001	HEM	C3C-C2C	-2.44	1.37	1.40
2	C	5001	ACT	O-C	2.42	1.33	1.22
4	A	4000	NDP	C7N-C3N	2.40	1.53	1.48
4	C	4001	NDP	O4B-C1B	2.30	1.44	1.41
3	C	3002	HEM	CBC-CAC	2.27	1.44	1.29
4	C	4001	NDP	C7N-C3N	2.26	1.53	1.48
3	D	3003	HEM	CAB-C3B	-2.24	1.41	1.47
3	A	3000	HEM	CBC-CAC	2.23	1.44	1.29
4	C	4001	NDP	P2B-O2B	2.20	1.63	1.59
4	A	4000	NDP	O4B-C1B	2.17	1.44	1.41
3	D	3003	HEM	CBC-CAC	2.15	1.43	1.29
3	D	3003	HEM	CHB-C1B	2.09	1.40	1.35
3	B	3001	HEM	CBC-CAC	2.07	1.43	1.29

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	5003	ACT	OXT-C-O	-6.92	96.54	122.05
2	A	5000	ACT	OXT-C-CH3	6.84	143.43	115.18
2	D	5003	ACT	OXT-C-CH3	6.81	143.33	115.18
2	A	5000	ACT	OXT-C-O	-4.71	104.69	122.05
2	C	5001	ACT	OXT-C-O	-4.55	105.27	122.05
4	C	4001	NDP	N3A-C2A-N1A	-4.31	121.94	128.68
4	A	4000	NDP	N3A-C2A-N1A	-4.20	122.12	128.68
2	B	5002	ACT	OXT-C-O	-3.30	109.91	122.05
3	A	3000	HEM	CMA-C3A-C4A	-3.09	123.72	128.46
2	A	5000	ACT	O-C-CH3	-2.97	110.77	122.33
3	D	3003	HEM	C4C-CHD-C1D	2.88	126.36	122.56
4	C	4001	NDP	C4A-C5A-N7A	2.74	112.25	109.40
3	C	3002	HEM	C4B-CHC-C1C	2.68	126.10	122.56
3	C	3002	HEM	C4C-CHD-C1D	2.61	126.00	122.56
3	D	3003	HEM	CBA-CAA-C2A	-2.56	108.25	112.62
3	A	3000	HEM	CMC-C2C-C3C	2.50	129.36	124.68
3	D	3003	HEM	CMC-C2C-C3C	2.47	129.31	124.68
4	A	4000	NDP	C5A-C6A-N6A	2.45	124.07	120.35
3	B	3001	HEM	C4C-CHD-C1D	2.39	125.71	122.56
3	B	3001	HEM	CMA-C3A-C4A	-2.39	124.80	128.46
3	C	3002	HEM	CMC-C2C-C3C	2.35	129.07	124.68
3	A	3000	HEM	C4B-CHC-C1C	2.35	125.65	122.56
4	C	4001	NDP	C3D-C2D-C1D	2.30	105.79	101.43
4	C	4001	NDP	C5A-C6A-N1A	-2.29	115.16	120.35
3	D	3003	HEM	C4B-CHC-C1C	2.26	125.54	122.56
2	C	5001	ACT	OXT-C-CH3	2.24	124.42	115.18
3	A	3000	HEM	CMA-C3A-C2A	2.18	129.04	124.94
3	D	3003	HEM	C4B-C3B-C2B	-2.14	105.41	107.11
4	C	4001	NDP	O2B-P2B-O1X	-2.13	101.15	109.39
4	A	4000	NDP	C4A-C5A-N7A	2.13	111.62	109.40
3	B	3001	HEM	CMA-C3A-C2A	2.13	128.95	124.94
4	A	4000	NDP	C1B-N9A-C4A	-2.09	122.97	126.64
3	A	3000	HEM	C4C-CHD-C1D	2.09	125.31	122.56
4	C	4001	NDP	C2A-N1A-C6A	2.08	122.31	118.75
3	B	3001	HEM	CMC-C2C-C3C	2.08	128.57	124.68
4	A	4000	NDP	C5A-C6A-N1A	-2.07	115.66	120.35
4	A	4000	NDP	C2B-C3B-C4B	2.06	106.47	101.99
2	C	5001	ACT	O-C-CH3	2.01	130.16	122.33

There are no chirality outliers.

All (19) torsion outliers are listed below:

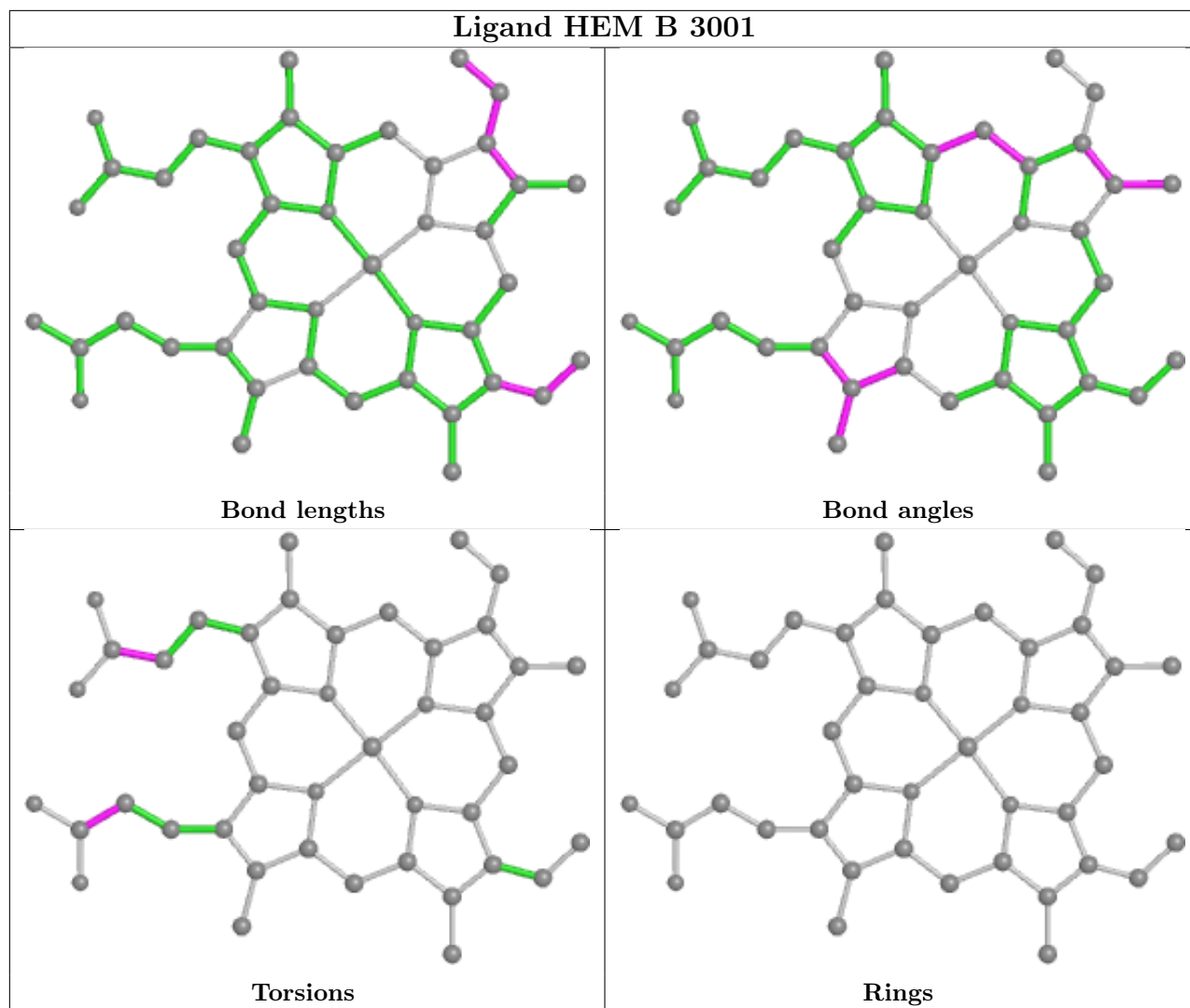
Mol	Chain	Res	Type	Atoms
4	A	4000	NDP	O4D-C1D-N1N-C6N
4	C	4001	NDP	O4D-C1D-N1N-C6N
4	A	4000	NDP	C2B-O2B-P2B-O2X
3	B	3001	HEM	CAD-CBD-CGD-O2D
3	B	3001	HEM	CAD-CBD-CGD-O1D
3	D	3003	HEM	CAD-CBD-CGD-O2D
3	C	3002	HEM	CAD-CBD-CGD-O2D
3	A	3000	HEM	CAD-CBD-CGD-O2D
3	D	3003	HEM	CAD-CBD-CGD-O1D
3	A	3000	HEM	CAD-CBD-CGD-O1D
3	C	3002	HEM	CAD-CBD-CGD-O1D
4	C	4001	NDP	C2B-O2B-P2B-O3X
4	A	4000	NDP	O4B-C4B-C5B-O5B
4	C	4001	NDP	O4B-C4B-C5B-O5B
3	B	3001	HEM	CAA-CBA-CGA-O1A
3	A	3000	HEM	CAA-CBA-CGA-O1A
3	D	3003	HEM	CAA-CBA-CGA-O1A
3	A	3000	HEM	CAA-CBA-CGA-O2A
3	C	3002	HEM	CAA-CBA-CGA-O1A

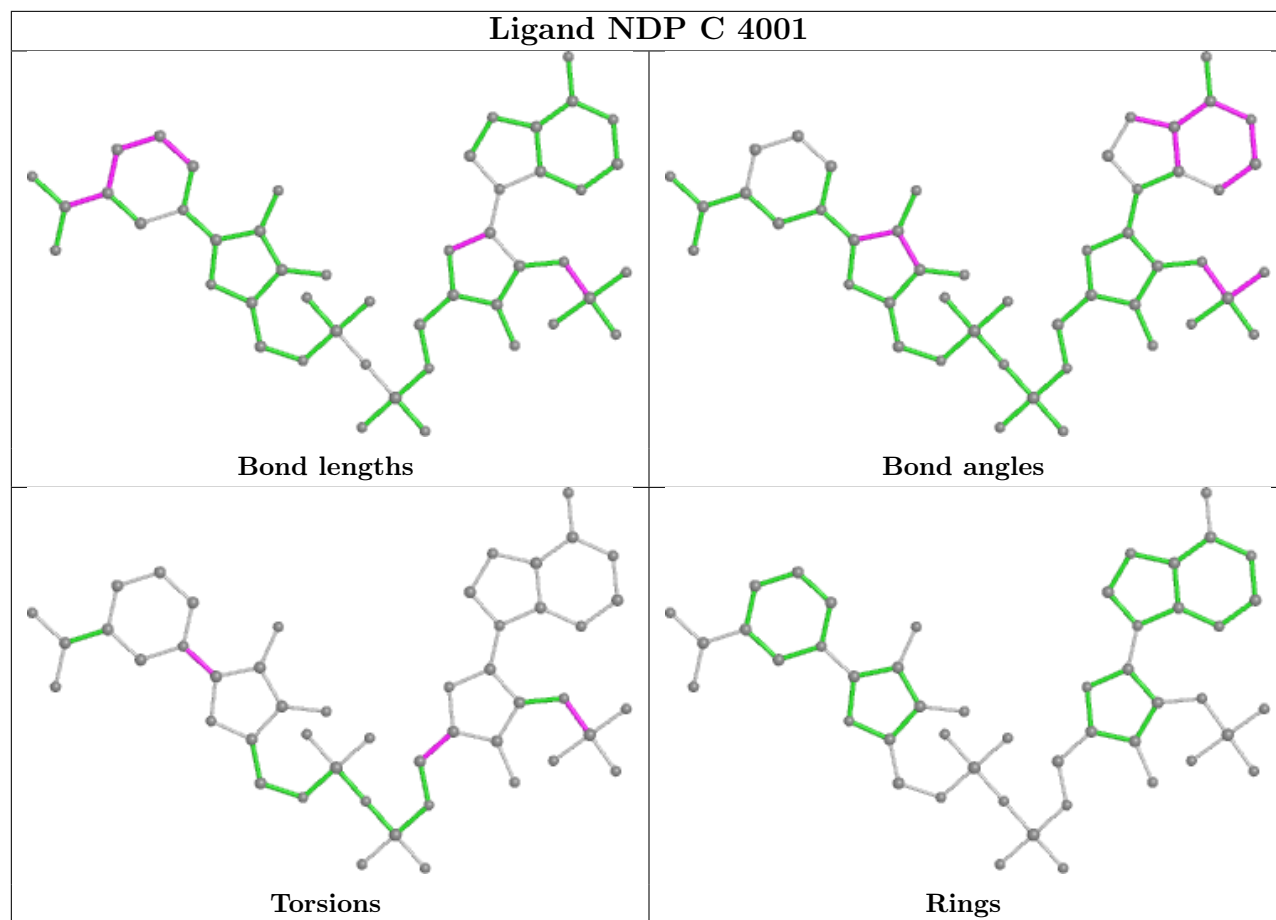
There are no ring outliers.

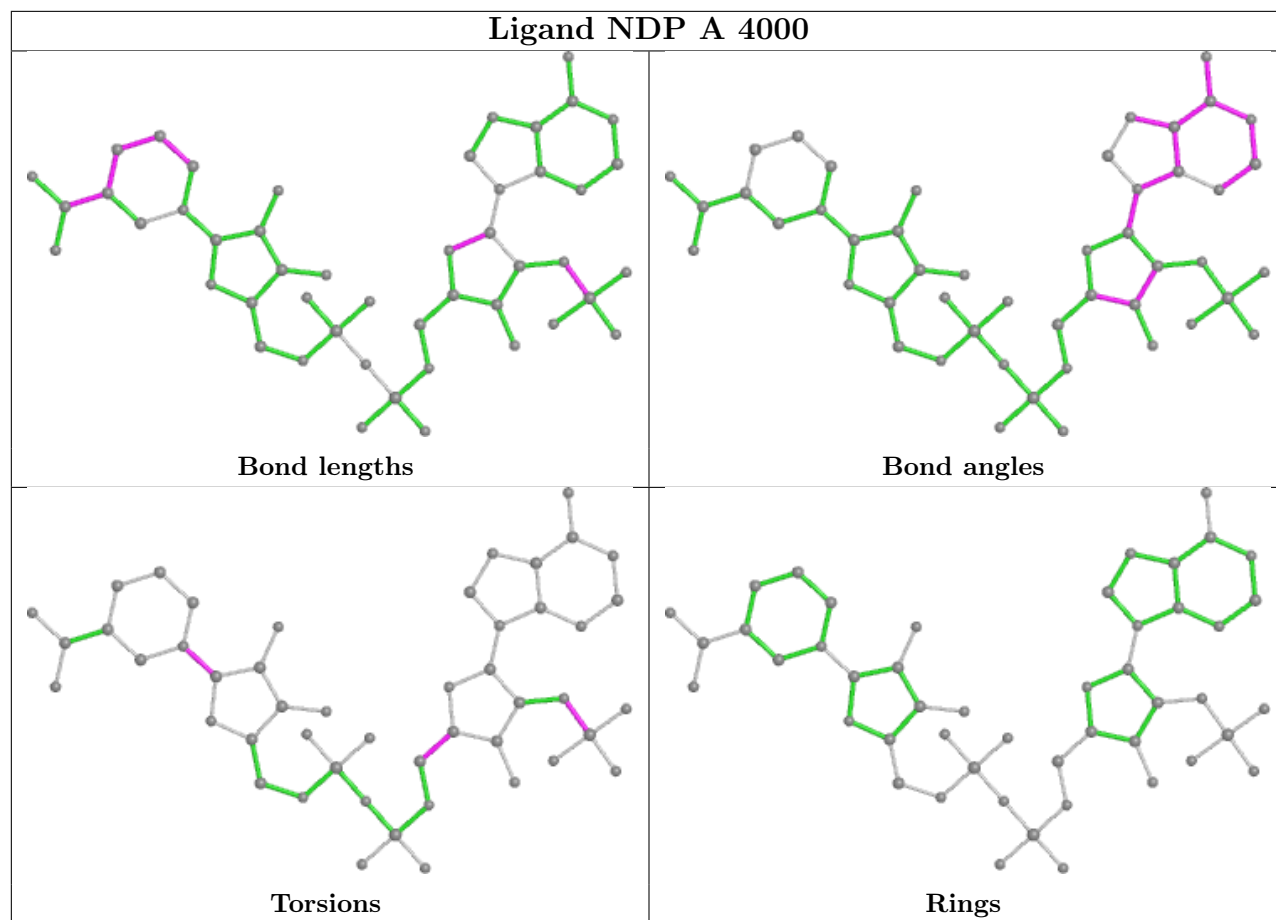
3 monomers are involved in 5 short contacts:

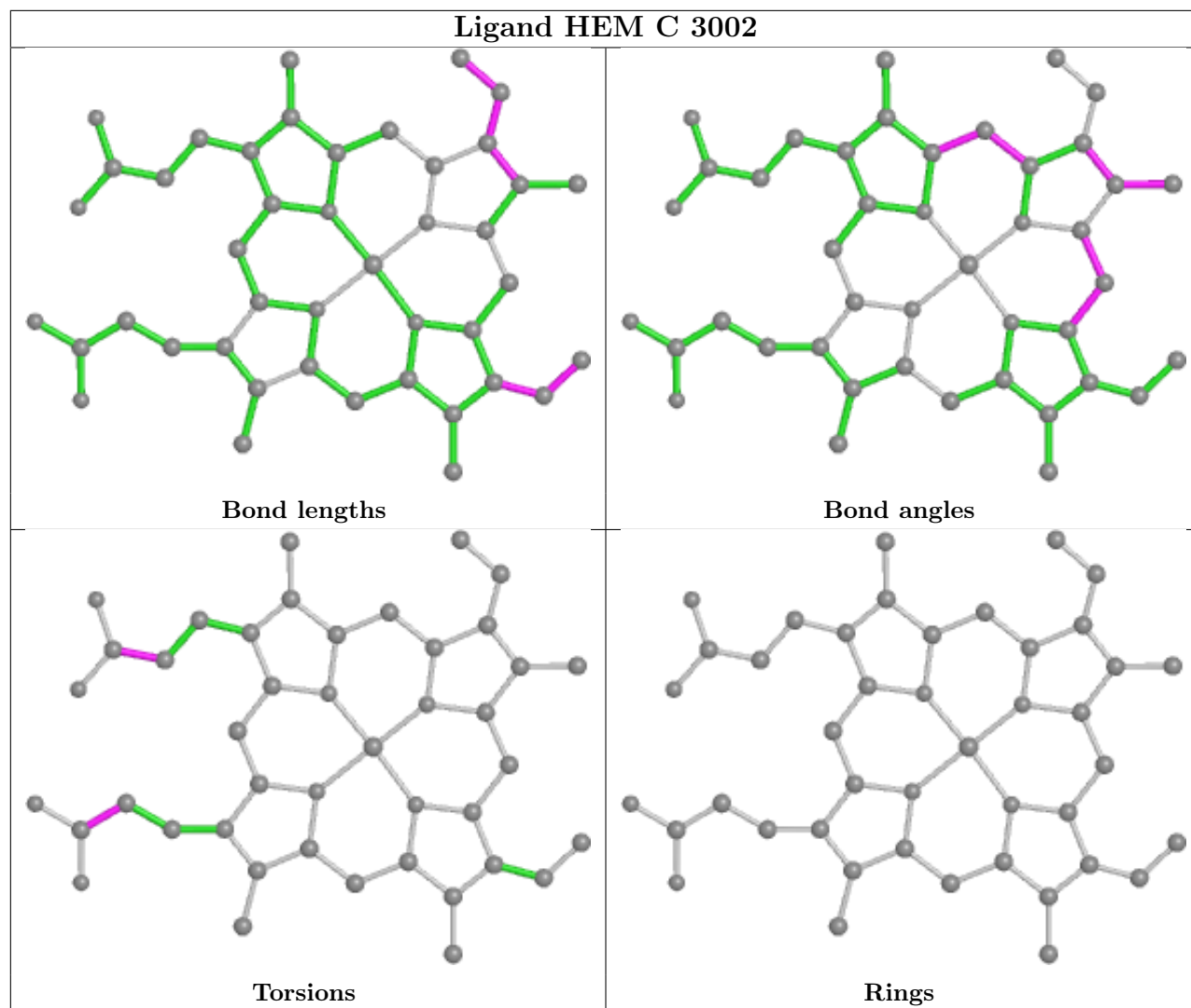
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	5001	ACT	1	0
2	D	5003	ACT	1	0
2	B	5002	ACT	3	0

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

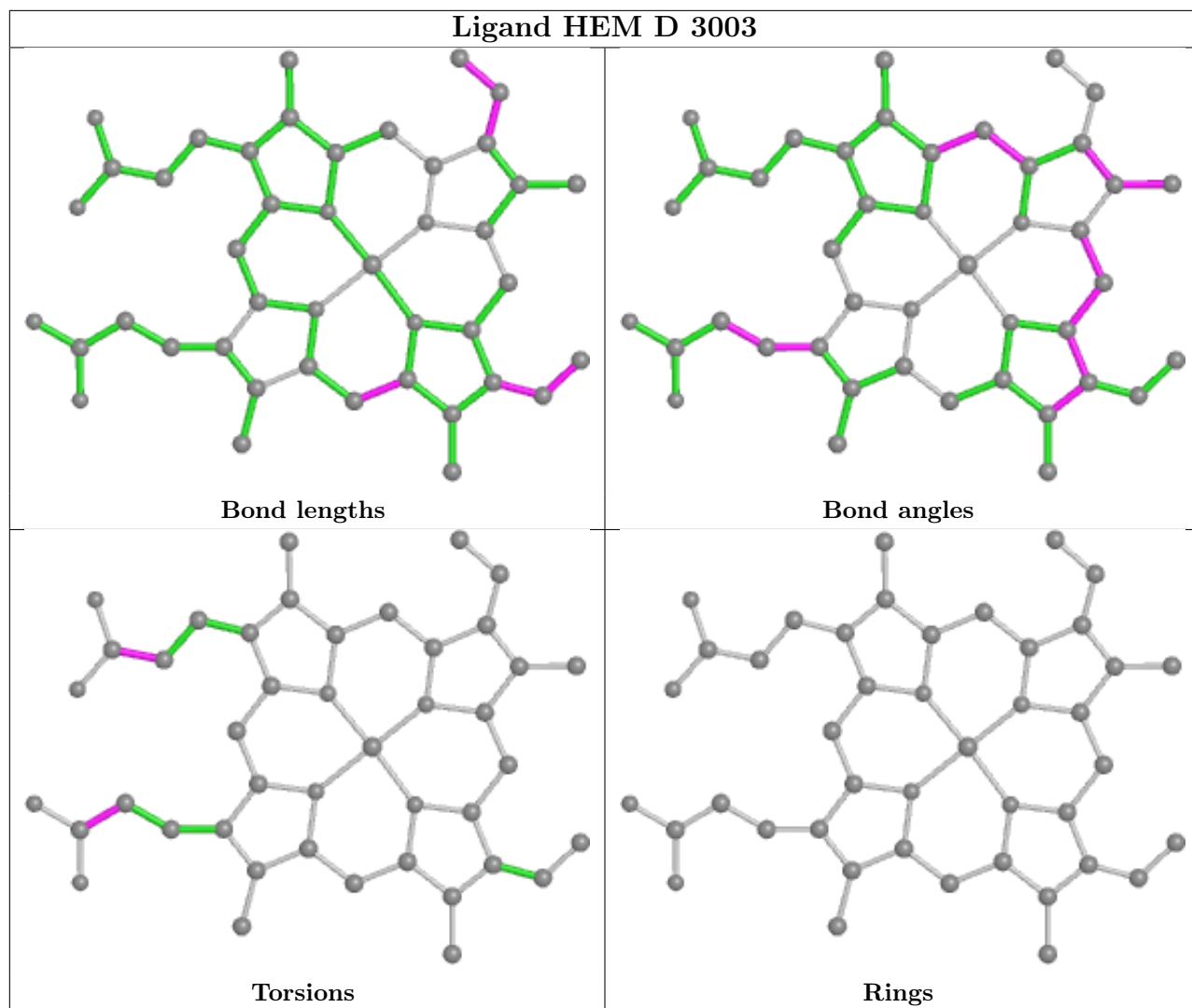


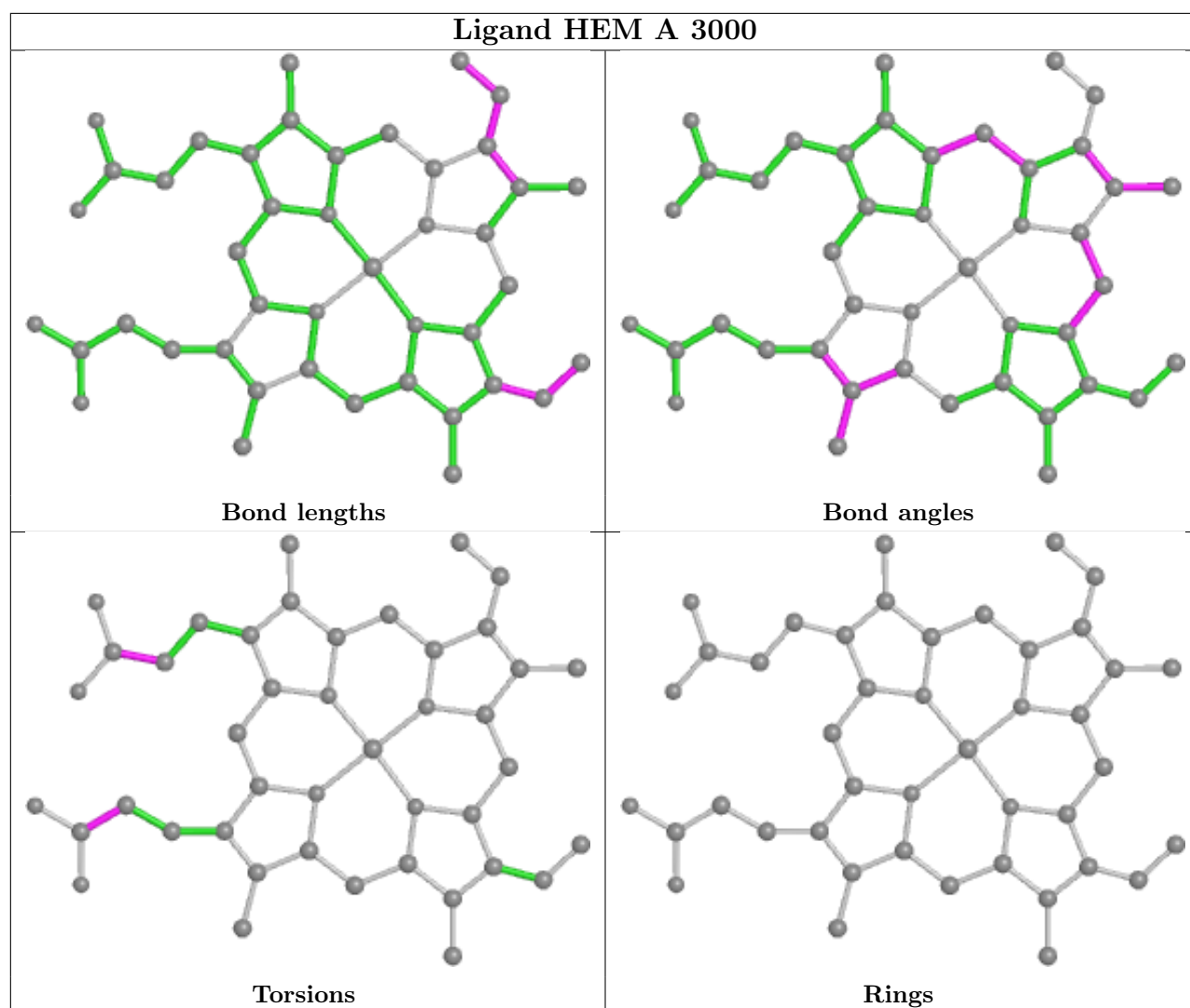












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	497/497 (100%)	-0.14	15 (3%)	50	55	6, 14, 26, 36	2 (0%)
1	B	497/497 (100%)	-0.18	15 (3%)	50	55	4, 13, 24, 36	0
1	C	497/497 (100%)	-0.17	15 (3%)	50	55	9, 14, 25, 35	0
1	D	497/497 (100%)	-0.20	13 (2%)	56	61	9, 13, 26, 32	0
All	All	1988/1988 (100%)	-0.17	58 (2%)	51	56	4, 14, 25, 36	2 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	21	ALA	9.3
1	B	21	ALA	8.3
1	C	21	ALA	6.7
1	D	21	ALA	6.6
1	B	20	ALA	6.1
1	A	500	TYR	5.1
1	C	500	TYR	4.9
1	C	20	ALA	4.4
1	A	20	ALA	4.0
1	D	20	ALA	3.6
1	B	305	HIS	3.6
1	A	394	MET	3.6
1	A	499	LYS	3.3
1	C	22	GLN	3.2
1	B	394	MET	3.1
1	D	500	TYR	3.1
1	D	499	LYS	2.9
1	A	18	GLN	2.9
1	D	394	MET	2.9
1	C	291	THR	2.9
1	A	395	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	226	ASN	2.8
1	D	426	SER	2.8
1	B	500	TYR	2.8
1	B	395	GLN	2.7
1	C	501	ASN	2.6
1	D	18	GLN	2.6
1	B	306	LYS	2.6
1	B	18	GLN	2.5
1	D	423	ILE	2.5
1	D	226	ASN	2.5
1	C	306	LYS	2.5
1	A	501	ASN	2.4
1	B	287	ASN	2.4
1	C	287	ASN	2.3
1	B	22	GLN	2.3
1	A	119	GLU	2.3
1	A	396	ASP	2.3
1	B	499	LYS	2.3
1	C	18	GLN	2.2
1	C	499	LYS	2.2
1	C	424	GLN	2.2
1	A	423	ILE	2.2
1	A	306	LYS	2.2
1	A	371	LEU	2.2
1	B	19	ARG	2.2
1	A	23	LYS	2.1
1	A	424	GLN	2.1
1	C	19	ARG	2.1
1	B	291	THR	2.1
1	D	305	HIS	2.1
1	D	424	GLN	2.1
1	C	395	GLN	2.0
1	D	291	THR	2.0
1	C	226	ASN	2.0
1	B	396	ASP	2.0
1	D	395	GLN	2.0
1	C	394	MET	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 [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

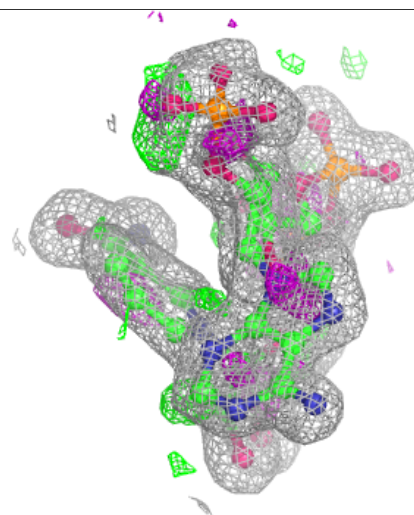
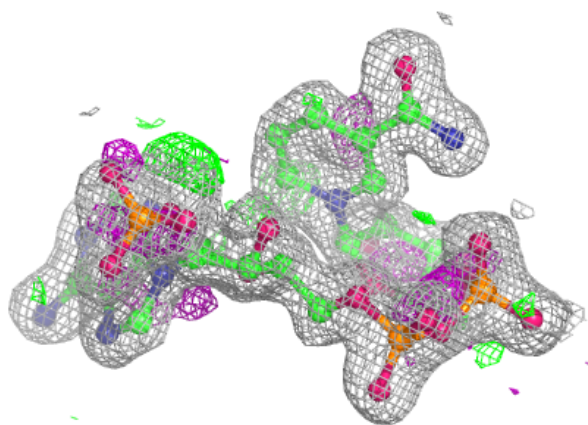
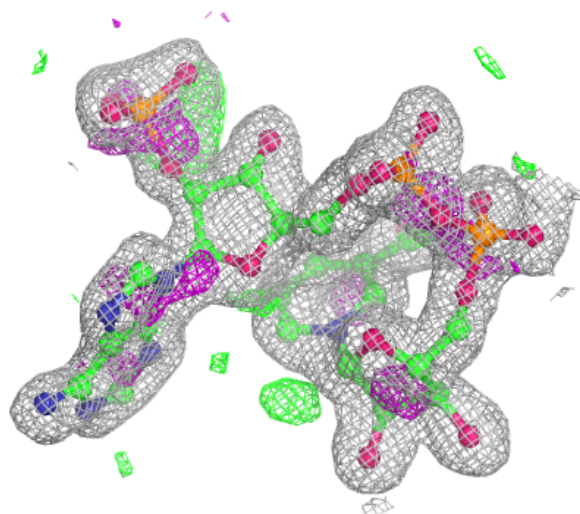
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ACT	A	5000	4/4	0.85	0.12	34,35,35,35	0
2	ACT	D	5003	4/4	0.88	0.12	33,33,34,34	0
2	ACT	C	5001	4/4	0.89	0.12	33,33,33,34	0
4	NDP	A	4000	48/48	0.90	0.14	24,30,35,35	0
2	ACT	B	5002	4/4	0.92	0.09	31,32,32,32	0
4	NDP	C	4001	48/48	0.94	0.10	18,23,35,36	0
3	HEM	D	3003	43/43	0.98	0.08	8,10,10,12	0
3	HEM	A	3000	43/43	0.98	0.07	9,11,12,12	0
3	HEM	C	3002	43/43	0.98	0.06	8,9,11,12	0
3	HEM	B	3001	43/43	0.99	0.07	8,9,10,11	0

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

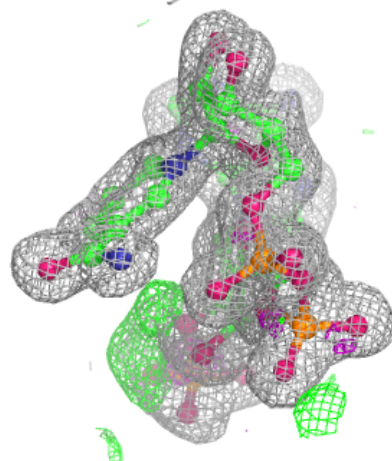
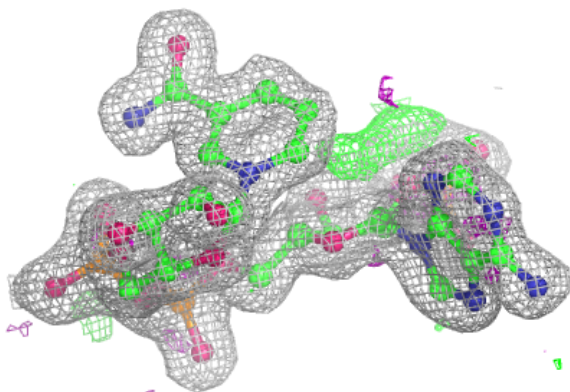
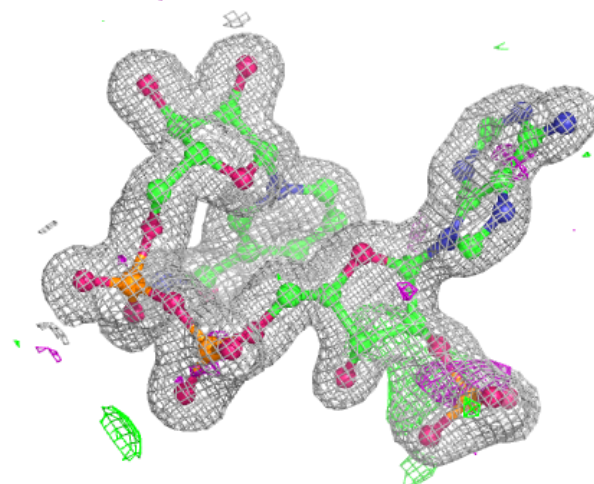
**Electron density around NDP A 4000:**

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



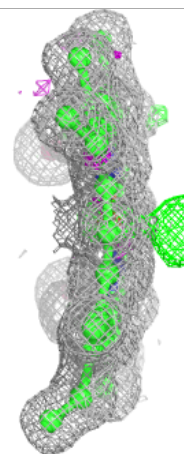
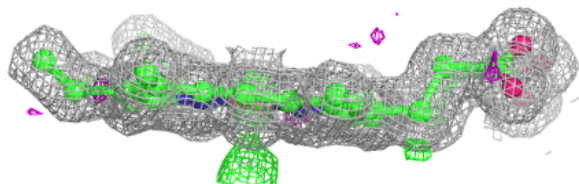
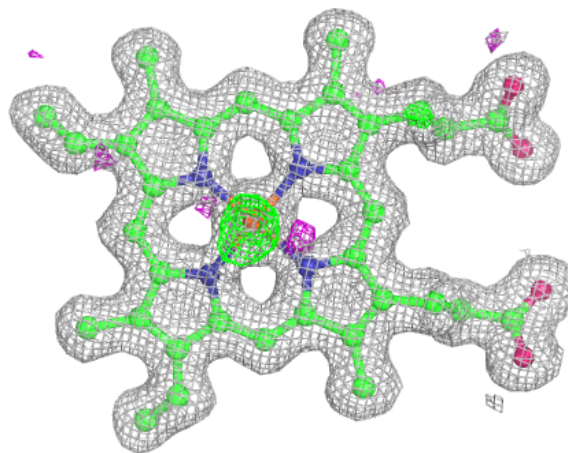
**Electron density around NDP C 4001:**

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



**Electron density around HEM D 3003:**

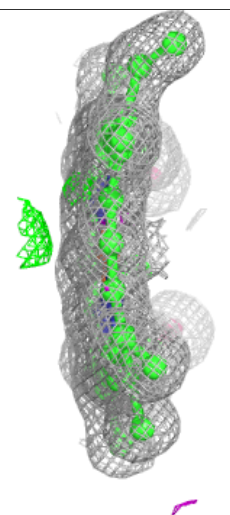
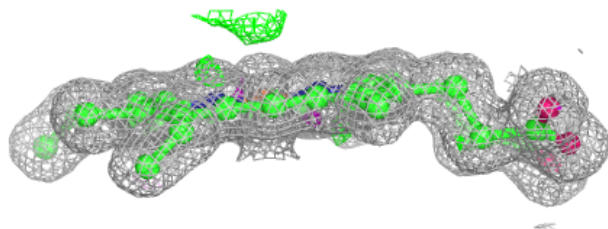
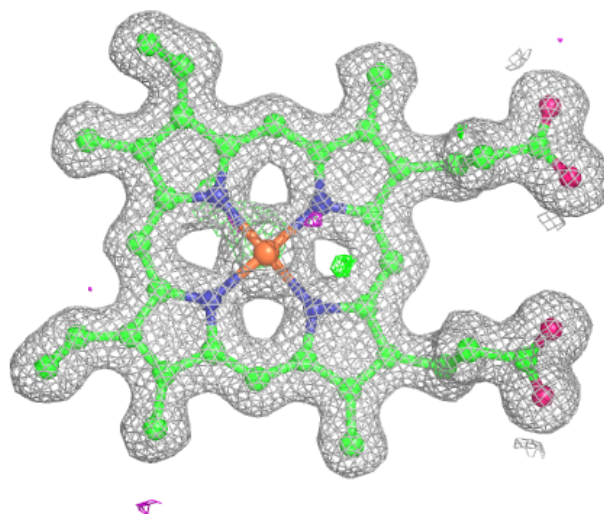
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





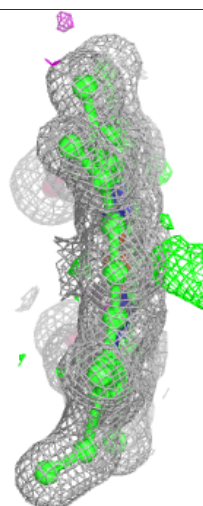
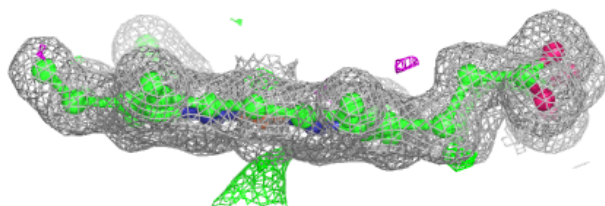
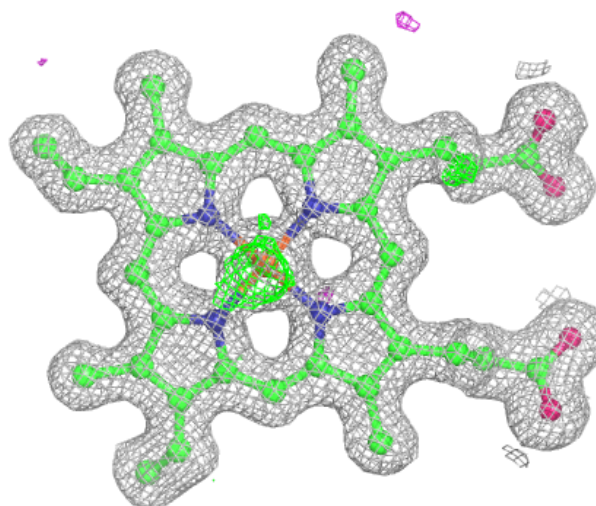
**Electron density around HEM A 3000:**

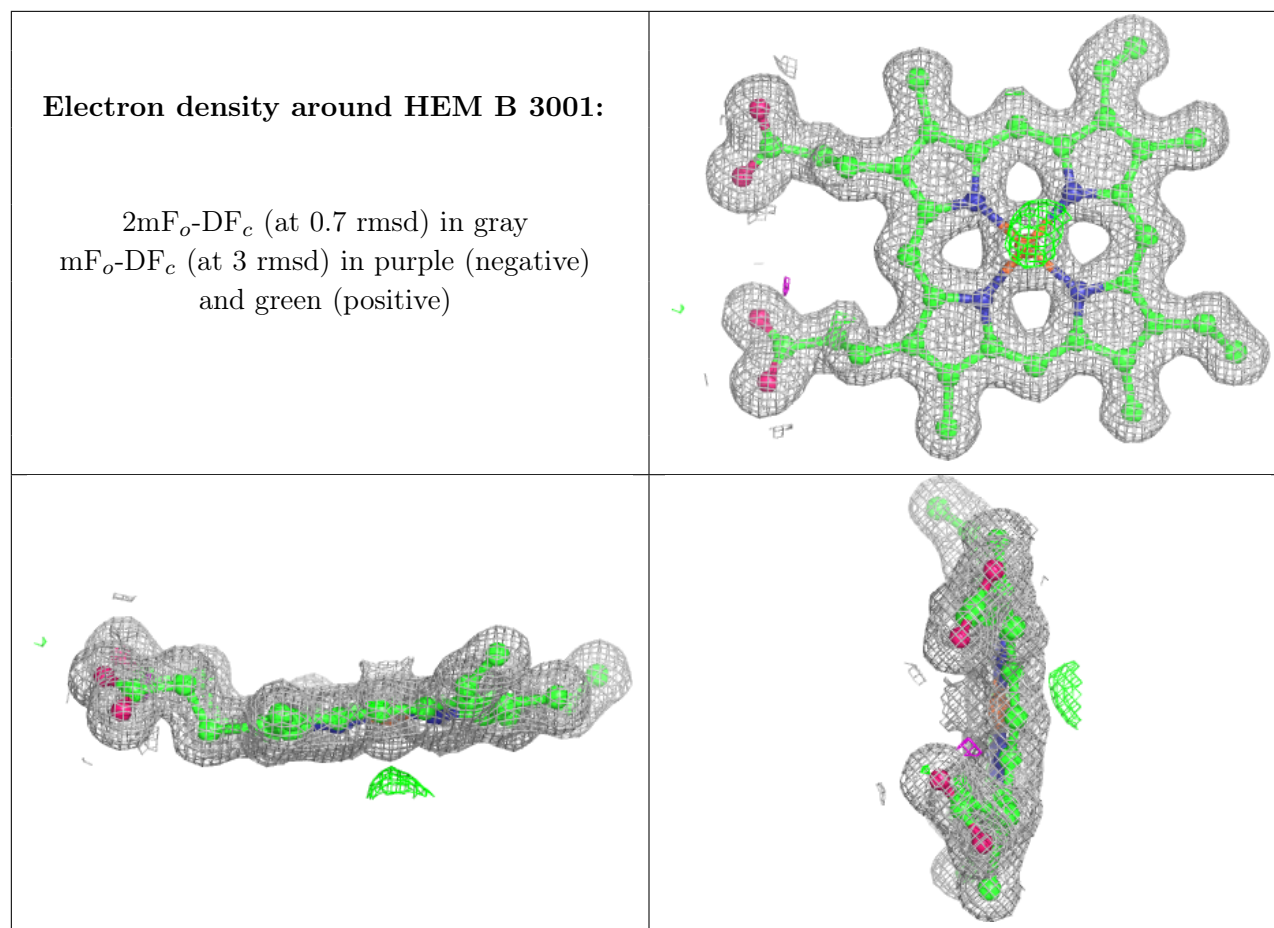
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM C 3002:**

$2mF_o-DF_c$  (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.