



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 09:18 pm BST

PDB ID : 4AUM  
Title : Crystal structure, recombinant expression and mutagenesis studies of the bi-functional catalase-phenol oxidase from *Scytalidium thermophilum*  
Authors : Yuzugullu, Y.; Trinh, C.H.; Smith, M.A.; Pearson, A.R.; Phillips, S.E.V.; Sutay Kocabas, D.; Bakir, U.; Ogel, Z.B.; McPherson, M.J.  
Deposited on : 2012-05-18  
Resolution : 1.40 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.

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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 : 2.11  
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) : 2.11

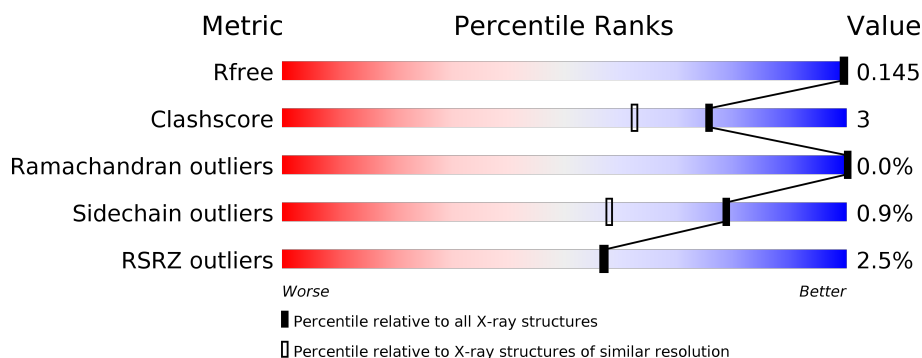
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.40 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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 on 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	719	<div> <div>88%</div> <div>5%</div> <div>6%</div> </div>
1	B	719	<div> <div>88%</div> <div>5%</div> <div>6%</div> </div>
1	C	719	<div> <div>3%</div> <div>88%</div> <div>5%</div> <div>7%</div> </div>
1	D	719	<div> <div>4%</div> <div>88%</div> <div>5%</div> <div>7%</div> </div>

## 2 Entry composition i

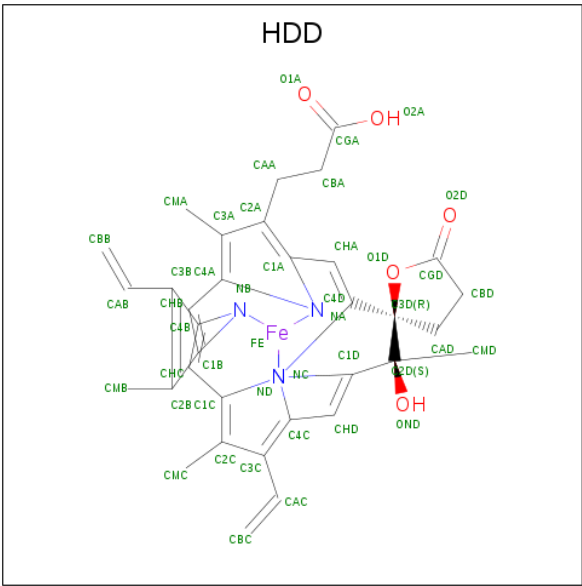
There are 5 unique types of molecules in this entry. The entry contains 24907 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-PHENOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	673	Total	C	N	O	S	0	48	0
			5587	3526	976	1072	13			
1	B	673	Total	C	N	O	S	0	47	0
			5590	3526	980	1072	12			
1	C	671	Total	C	N	O	S	0	45	0
			5545	3502	972	1057	14			
1	D	671	Total	C	N	O	S	0	41	0
			5520	3489	966	1051	14			

- Molecule 2 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (three-letter code: HDD) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		
2	B	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		

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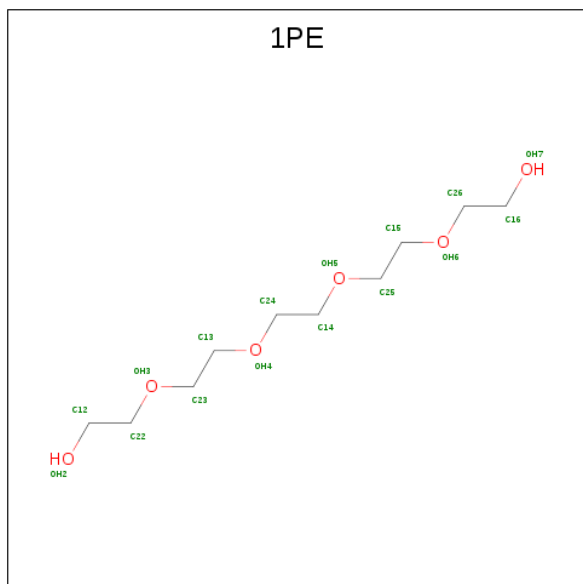
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		
2	D	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Ca	0	0
			3	3		
3	A	3	Total	Ca	0	0
			3	3		
3	D	2	Total	Ca	0	0
			2	2		
3	C	2	Total	Ca	0	0
			2	2		

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			16	10	6		

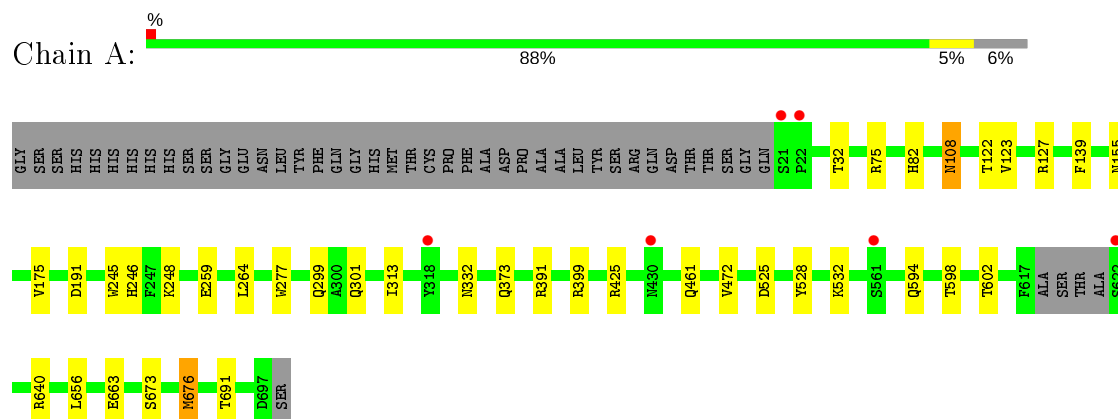
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	772	Total 772	O 772	0	0
5	B	694	Total 694	O 694	0	0
5	C	524	Total 524	O 524	0	0
5	D	473	Total 473	O 473	0	0

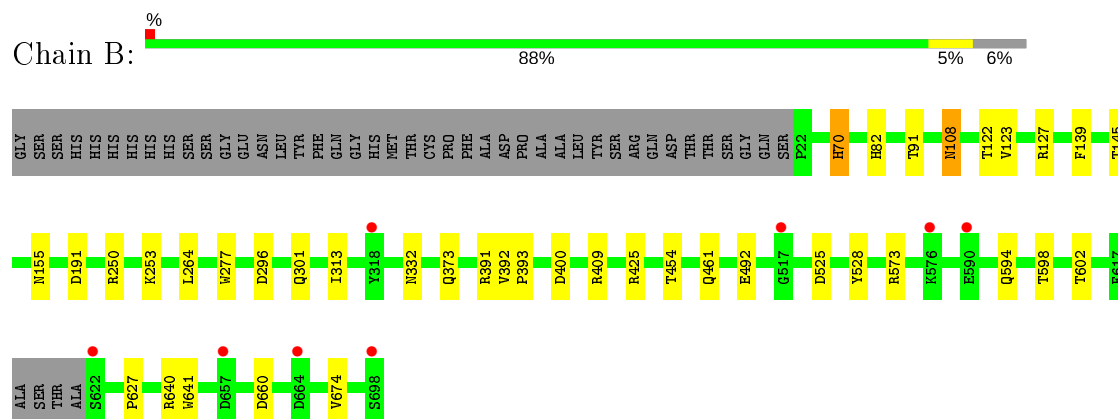
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

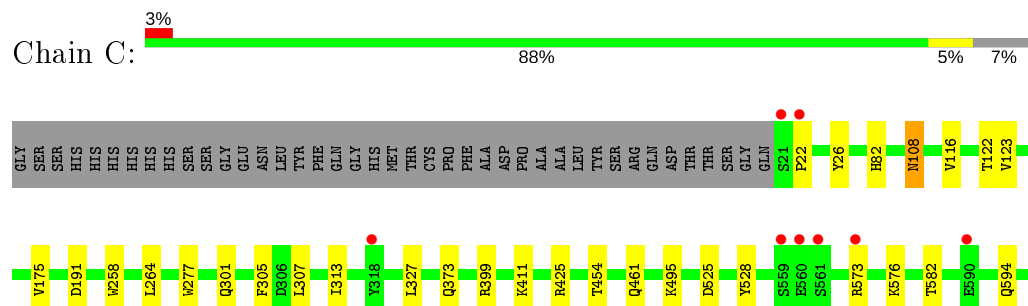
#### • Molecule 1: CATALASE-PHENOL OXIDASE

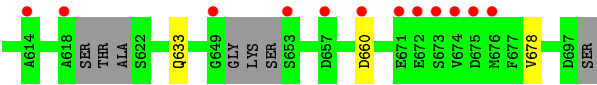


#### • Molecule 1: CATALASE-PHENOL OXIDASE

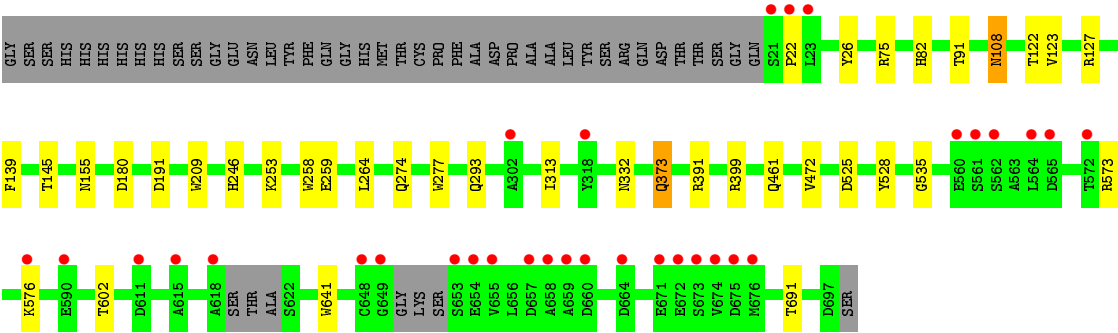
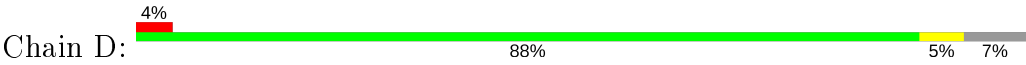


#### • Molecule 1: CATALASE-PHENOL OXIDASE





● Molecule 1: CATALASE-PHENOL OXIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	201.42Å 121.45Å 125.21Å 90.00° 115.51° 90.00°	Depositor
Resolution (Å)	113.00 – 1.40 29.32 – 1.40	Depositor EDS
% Data completeness (in resolution range)	95.2 (113.00-1.40) 95.2 (29.32-1.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.96 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.118 , 0.145 0.117 , 0.145	Depositor DCC
$R_{free}$ test set	25334 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.1	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	24907	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.82 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0392e-03.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, HDD, 1PE

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	0.57	1/5794 (0.0%)	0.68	2/7862 (0.0%)
1	B	0.55	1/5788 (0.0%)	0.66	0/7853
1	C	0.57	2/5751 (0.0%)	0.68	1/7803 (0.0%)
1	D	0.56	3/5714 (0.1%)	0.67	2/7754 (0.0%)
All	All	0.56	7/23047 (0.0%)	0.67	5/31272 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	209	TRP	CD2-CE2	5.33	1.47	1.41
1	D	258	TRP	CD2-CE2	5.24	1.47	1.41
1	A	245	TRP	CD2-CE2	5.20	1.47	1.41
1	B	641	TRP	CD2-CE2	5.14	1.47	1.41
1	D	641	TRP	CD2-CE2	5.12	1.47	1.41
1	C	258	TRP	CD2-CE2	5.08	1.47	1.41
1	C	277	TRP	CD2-CE2	5.04	1.47	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	A	399	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	D	399	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	C	399	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	D	75	ARG	NE-CZ-NH2	-5.34	117.63	120.30

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	5587	0	5397	38	0
1	B	5590	0	5399	41	0
1	C	5545	0	5367	31	0
1	D	5520	0	5342	29	0
2	A	44	0	31	2	0
2	B	44	0	31	1	0
2	C	44	0	31	1	0
2	D	44	0	31	1	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	16	0	22	0	0
5	A	772	0	0	23	0
5	B	694	0	0	21	0
5	C	524	0	0	8	0
5	D	473	0	0	5	0
All	All	24907	0	21651	135	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 (135) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409[B]:ARG:HH11	1:B:409[B]:ARG:HG2	1.09	1.13
1:A:259[A]:GLU:HG3	5:A:2357:HOH:O	1.49	1.11
5:A:2109:HOH:O	1:C:127[B]:ARG:NH2	1.83	1.08
1:A:676[A]:MET:HE1	5:A:2752:HOH:O	1.57	1.02
1:B:127[A]:ARG:NH2	5:B:2171:HOH:O	1.93	1.01
5:B:2106:HOH:O	1:D:127[B]:ARG:NH1	1.83	1.01
1:B:627:PRO:HB3	1:D:259[B]:GLU:OE2	1.59	1.01
1:A:127[A]:ARG:NH2	5:A:2193:HOH:O	1.94	0.98
5:B:2106:HOH:O	1:D:127[B]:ARG:NH2	1.97	0.97
1:D:313:ILE:H	1:D:461:GLN:HE22	1.14	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127[A]:ARG:NH1	5:A:2193:HOH:O	2.00	0.95
5:B:2106:HOH:O	1:D:127[B]:ARG:CZ	2.16	0.93
1:C:313:ILE:H	1:C:461:GLN:HE22	1.16	0.92
5:A:2109:HOH:O	1:C:127[B]:ARG:NH1	2.03	0.91
1:B:127[A]:ARG:NH1	5:B:2171:HOH:O	2.00	0.91
1:A:313:ILE:H	1:A:461:GLN:HE22	1.17	0.90
1:B:313:ILE:H	1:B:461:GLN:HE22	1.16	0.90
1:B:409[B]:ARG:HG2	1:B:409[B]:ARG:NH1	1.86	0.87
5:A:2109:HOH:O	1:C:127[B]:ARG:CZ	2.18	0.85
1:B:70:HIS:CE1	5:B:2084:HOH:O	2.31	0.83
1:A:127[A]:ARG:CZ	5:A:2193:HOH:O	2.22	0.82
1:B:627:PRO:CB	1:D:259[B]:GLU:OE2	2.28	0.81
1:B:91[B]:THR:HG22	5:B:2125:HOH:O	1.81	0.80
1:C:573[A]:ARG:HG2	1:C:678:VAL:HG21	1.64	0.79
1:A:425[B]:ARG:CZ	5:A:2534:HOH:O	2.31	0.78
1:A:676[A]:MET:CE	5:A:2752:HOH:O	2.23	0.78
1:A:640[A]:ARG:HG2	5:A:2363:HOH:O	1.86	0.76
1:D:91[B]:THR:HG22	5:D:2051:HOH:O	1.87	0.75
1:B:127[A]:ARG:CZ	5:B:2171:HOH:O	2.22	0.74
1:D:264:LEU:HG	1:D:602:THR:HB	1.70	0.74
1:B:264:LEU:HG	1:B:602:THR:HB	1.69	0.73
1:D:246[A]:HIS:CD2	5:D:2203:HOH:O	2.42	0.72
1:A:264:LEU:HG	1:A:602:THR:HB	1.72	0.72
1:A:425[B]:ARG:NH1	5:A:2534:HOH:O	2.25	0.70
1:D:573:ARG:HH11	1:D:573:ARG:HG3	1.55	0.70
1:A:127[B]:ARG:NH1	5:A:2195:HOH:O	2.24	0.68
1:C:411[B]:LYS:HE3	5:C:2327:HOH:O	1.94	0.68
1:A:640[A]:ARG:CG	5:A:2363:HOH:O	2.42	0.67
1:B:127[B]:ARG:NH1	5:B:2174:HOH:O	2.27	0.66
1:C:495[B]:LYS:HE2	5:C:2164:HOH:O	1.94	0.66
1:C:576:LYS:HG3	5:C:2470:HOH:O	1.97	0.65
5:B:2169:HOH:O	1:D:127[A]:ARG:NH1	2.29	0.65
1:C:264:LEU:HG	1:C:602:THR:HB	1.78	0.64
1:D:373:GLN:HA	1:D:373:GLN:HE21	1.62	0.64
1:B:392[B]:VAL:HG13	1:B:393:PRO:HD2	1.80	0.64
1:B:640[B]:ARG:HG2	5:B:2318:HOH:O	2.00	0.61
1:A:373:GLN:HE21	1:A:373:GLN:HA	1.66	0.60
1:B:627:PRO:CG	1:D:259[B]:GLU:OE2	2.49	0.60
1:C:373:GLN:HE21	1:C:373:GLN:HA	1.67	0.60
1:B:373:GLN:HA	1:B:373:GLN:HE21	1.66	0.60
1:C:411[B]:LYS:HE2	1:D:180:ASP:OD2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:PRO:O	1:C:26:TYR:HD2	1.85	0.59
1:D:313:ILE:N	1:D:461:GLN:HE22	1.93	0.57
1:B:70:HIS:HE1	5:B:2084:HOH:O	1.74	0.57
1:A:656:LEU:HD12	1:A:663[A]:GLU:HG3	1.86	0.57
1:C:313:ILE:N	1:C:461:GLN:HE22	1.97	0.57
1:A:656:LEU:CD1	1:A:663[A]:GLU:HG3	2.35	0.56
1:C:582:THR:HG21	1:C:594[A]:GLN:HE21	1.70	0.56
1:D:22:PRO:O	1:D:26:TYR:HD2	1.89	0.56
1:A:175[B]:VAL:CG1	5:A:2267:HOH:O	2.53	0.56
5:A:2191:HOH:O	1:C:127[A]:ARG:NH1	2.38	0.56
1:B:313:ILE:N	1:B:461:GLN:HE22	1.97	0.56
1:B:108:ASN:C	1:B:108:ASN:HD22	2.09	0.55
1:D:391[B]:ARG:NE	5:D:2294:HOH:O	2.40	0.55
1:A:313:ILE:N	1:A:461:GLN:HE22	1.97	0.55
1:B:409[B]:ARG:CG	1:B:409[B]:ARG:NH1	2.64	0.55
1:A:108:ASN:HD22	1:A:108:ASN:C	2.11	0.54
1:C:411[B]:LYS:CE	5:C:2327:HOH:O	2.54	0.52
1:C:108:ASN:HD22	1:C:108:ASN:C	2.10	0.52
1:A:32:THR:HG22	5:A:2013:HOH:O	2.09	0.52
1:B:492[A]:GLU:HG2	5:B:2545:HOH:O	2.10	0.52
1:B:640[B]:ARG:CG	5:B:2318:HOH:O	2.57	0.51
1:D:108:ASN:HD22	1:D:108:ASN:C	2.13	0.51
1:B:425[B]:ARG:CZ	5:B:2470:HOH:O	2.59	0.50
1:D:91[B]:THR:HG23	5:D:2049:HOH:O	2.11	0.50
1:B:594[A]:GLN:HG3	1:B:598:THR:OG1	2.12	0.50
1:D:274[B]:GLN:CD	5:D:2226:HOH:O	2.51	0.49
1:B:253:LYS:HG2	5:B:2275:HOH:O	2.12	0.49
1:C:425[A]:ARG:NH1	5:C:2340:HOH:O	2.45	0.49
1:B:573[B]:ARG:HG3	1:B:674:VAL:CG1	2.43	0.49
1:B:91[B]:THR:HG23	5:B:2126:HOH:O	2.12	0.49
1:A:472[A]:VAL:HG11	1:A:691:THR:HB	1.95	0.47
1:C:525:ASP:HA	1:C:528:TYR:CD2	2.49	0.47
1:C:495[B]:LYS:HE3	5:C:2415:HOH:O	2.14	0.47
1:A:425[B]:ARG:NH2	5:A:2534:HOH:O	2.46	0.46
1:D:525:ASP:HA	1:D:528:TYR:CD2	2.50	0.46
1:D:82:HIS:CE1	1:D:123:VAL:HG22	2.50	0.46
1:D:246[A]:HIS:CE1	1:D:293:GLN:OE1	2.69	0.46
1:B:525:ASP:HA	1:B:528:TYR:CD2	2.51	0.45
1:C:175[B]:VAL:HG11	5:C:2108:HOH:O	2.15	0.45
1:C:301:GLN:NE2	1:C:454:THR:HG21	2.31	0.45
1:B:82:HIS:CE1	1:B:123:VAL:HG22	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:472[A]:VAL:HG11	1:D:691:THR:HB	1.98	0.45
1:B:301:GLN:NE2	1:B:454:THR:HG21	2.32	0.44
1:A:640[B]:ARG:NH1	5:A:2717:HOH:O	2.50	0.44
1:A:155:ASN:CG	2:A:900:HDD:HMB2	2.38	0.44
1:A:259[A]:GLU:CG	5:A:2357:HOH:O	2.29	0.44
1:B:277:TRP:CH2	1:B:332:ASN:HB3	2.53	0.44
1:D:82:HIS:HA	1:D:122:THR:O	2.18	0.44
1:C:82:HIS:CE1	1:C:123:VAL:HG22	2.53	0.43
1:A:246[B]:HIS:CE1	1:A:248[B]:LYS:HD3	2.53	0.43
1:A:594[A]:GLN:HG3	1:A:598:THR:OG1	2.18	0.43
1:B:155:ASN:CG	2:B:900:HDD:HMB2	2.39	0.43
1:B:573[B]:ARG:HG3	1:B:674:VAL:HG12	1.99	0.43
1:D:573:ARG:HG3	1:D:573:ARG:NH1	2.27	0.43
1:C:594[A]:GLN:HG3	1:C:598:THR:OG1	2.19	0.42
1:C:82:HIS:HA	1:C:122:THR:O	2.19	0.42
1:B:250:ARG:HD3	5:B:2304:HOH:O	2.18	0.42
1:D:253[A]:LYS:NZ	1:D:535:GLY:O	2.53	0.42
1:C:116:VAL:HG21	1:C:327:LEU:HD11	2.02	0.42
1:B:573[B]:ARG:HD3	5:B:2603:HOH:O	2.20	0.42
1:C:155:ASN:CG	2:C:900:HDD:HMB2	2.40	0.42
1:B:391[B]:ARG:HA	1:B:391[B]:ARG:HD3	1.91	0.41
1:C:633[B]:GLN:OE1	5:C:2484:HOH:O	2.22	0.41
1:A:532:LYS:HE2	5:A:2590:HOH:O	2.19	0.41
1:B:82:HIS:HA	1:B:122:THR:O	2.20	0.41
1:D:277:TRP:CH2	1:D:332:ASN:HB3	2.55	0.41
1:A:525:ASP:HA	1:A:528:TYR:CD2	2.54	0.41
1:B:108:ASN:C	1:B:108:ASN:ND2	2.74	0.41
1:C:301:GLN:HE22	1:C:454:THR:HG21	1.86	0.41
1:B:373:GLN:HA	1:B:373:GLN:NE2	2.33	0.41
1:B:640[A]:ARG:NH1	5:B:2650:HOH:O	2.51	0.41
1:D:155:ASN:CG	2:D:900:HDD:HMB2	2.40	0.41
1:A:472[B]:VAL:HG23	5:A:2596:HOH:O	2.20	0.41
1:A:82:HIS:CE1	1:A:123:VAL:HG22	2.56	0.41
1:A:299:GLN:OE1	5:A:2411:HOH:O	2.21	0.41
1:A:673:SER:HB3	1:A:676[A]:MET:HB2	2.02	0.41
1:A:277:TRP:CH2	1:A:332:ASN:HB3	2.56	0.40
1:A:155:ASN:ND2	2:A:900:HDD:HMB2	2.36	0.40
1:C:305:PHE:CE1	1:C:307:LEU:HD23	2.56	0.40
1:A:391[A]:ARG:HD3	1:A:391[A]:ARG:HA	1.88	0.40
1:B:640[B]:ARG:NH1	5:B:2650:HOH:O	2.55	0.40
1:C:425[A]:ARG:HE	1:C:425[A]:ARG:HB3	1.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:HIS:HA	1:A:122:THR:O	2.22	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	717/719 (100%)	701 (98%)	16 (2%)	0	100	100
1	B	716/719 (100%)	700 (98%)	15 (2%)	1 (0%)	51	23
1	C	710/719 (99%)	695 (98%)	15 (2%)	0	100	100
1	D	706/719 (98%)	692 (98%)	14 (2%)	0	100	100
All	All	2849/2876 (99%)	2788 (98%)	60 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	400	ASP

### 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	606/596 (102%)	601 (99%)	5 (1%)	81	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	605/596 (102%)	598 (99%)	7 (1%)	71	47
1	C	600/596 (101%)	596 (99%)	4 (1%)	84	66
1	D	596/596 (100%)	590 (99%)	6 (1%)	76	53
All	All	2407/2384 (101%)	2385 (99%)	22 (1%)	78	58

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	139	PHE
1	A	191	ASP
1	A	676[A]	MET
1	A	676[B]	MET
1	B	70	HIS
1	B	108	ASN
1	B	139	PHE
1	B	145	THR
1	B	191	ASP
1	B	296	ASP
1	B	660	ASP
1	C	108	ASN
1	C	139	PHE
1	C	191	ASP
1	C	660	ASP
1	D	108	ASN
1	D	139	PHE
1	D	145	THR
1	D	191	ASP
1	D	373	GLN
1	D	576	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	167	GLN
1	A	373	GLN
1	A	375	ASN
1	A	461	GLN
1	B	108	ASN

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Mol	Chain	Res	Type
1	B	301	GLN
1	B	373	GLN
1	B	375	ASN
1	B	461	GLN
1	C	108	ASN
1	C	167	GLN
1	C	199	GLN
1	C	301	GLN
1	C	373	GLN
1	C	375	ASN
1	C	461	GLN
1	D	108	ASN
1	D	167	GLN
1	D	301	GLN
1	D	373	GLN
1	D	375	ASN
1	D	461	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 10 are monoatomic - leaving 5 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
4	1PE	A	1698	-	15,15,15	0.42	0	14,14,14	0.34	0
2	HDD	A	900	1,5	38,52,52	1.33	6 (15%)	28,89,89	2.27	8 (28%)
2	HDD	D	900	1,5	38,52,52	1.35	5 (13%)	28,89,89	2.15	9 (32%)
2	HDD	B	900	1,5	38,52,52	1.32	4 (10%)	28,89,89	2.17	7 (25%)
2	HDD	C	900	1,5	38,52,52	1.31	6 (15%)	28,89,89	2.01	9 (32%)

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
4	1PE	A	1698	-	-	1/13/13/13	-
2	HDD	A	900	1,5	-	0/3/89/89	0/1/9/9
2	HDD	D	900	1,5	-	0/3/89/89	0/1/9/9
2	HDD	B	900	1,5	-	0/3/89/89	0/1/9/9
2	HDD	C	900	1,5	-	0/3/89/89	0/1/9/9

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	HDD	O1D-CGD	3.82	1.42	1.35
2	D	900	HDD	O1D-CGD	3.72	1.41	1.35
2	B	900	HDD	O1D-CGD	3.69	1.41	1.35
2	C	900	HDD	O1D-CGD	3.40	1.41	1.35
2	D	900	HDD	C3C-C2C	3.26	1.44	1.40
2	C	900	HDD	C3C-C2C	3.24	1.44	1.40
2	B	900	HDD	C3C-C2C	3.12	1.44	1.40
2	C	900	HDD	C3B-C2B	3.07	1.44	1.40
2	B	900	HDD	C3B-C2B	2.92	1.44	1.40
2	D	900	HDD	C3B-C2B	2.91	1.44	1.40
2	A	900	HDD	C3B-C2B	2.63	1.44	1.40
2	B	900	HDD	C2A-C3A	2.58	1.45	1.37
2	A	900	HDD	C3C-C2C	2.45	1.43	1.40
2	A	900	HDD	C4C-CHD	2.38	1.47	1.41
2	A	900	HDD	C2A-C3A	2.26	1.44	1.37
2	C	900	HDD	C2A-C3A	2.20	1.44	1.37
2	C	900	HDD	C1A-CHA	2.17	1.47	1.41
2	A	900	HDD	C1A-CHA	2.13	1.46	1.41
2	D	900	HDD	C1A-CHA	2.05	1.46	1.41
2	C	900	HDD	C4C-CHD	2.03	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	900	HDD	C2A-C3A	2.01	1.43	1.37

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	HDD	C4A-C3A-C2A	-7.01	102.12	107.00
2	B	900	HDD	C4A-C3A-C2A	-6.93	102.18	107.00
2	D	900	HDD	C4A-C3A-C2A	-6.74	102.31	107.00
2	C	900	HDD	C4A-C3A-C2A	-5.94	102.86	107.00
2	A	900	HDD	CAA-CBA-CGA	-4.80	104.62	112.67
2	B	900	HDD	CAA-CBA-CGA	-4.42	105.25	112.67
2	D	900	HDD	CAA-CBA-CGA	-4.30	105.45	112.67
2	A	900	HDD	C2D-C1D-CHD	-4.10	117.52	124.28
2	D	900	HDD	C3C-C4C-NC	3.83	114.16	109.21
2	C	900	HDD	CAA-CBA-CGA	-3.66	106.53	112.67
2	C	900	HDD	C2D-C1D-CHD	-3.65	118.25	124.28
2	B	900	HDD	C3C-C4C-NC	3.39	113.59	109.21
2	B	900	HDD	C2D-C1D-CHD	-3.25	118.91	124.28
2	B	900	HDD	CMB-C2B-C3B	3.17	130.61	124.68
2	A	900	HDD	C3C-C4C-NC	3.10	113.21	109.21
2	D	900	HDD	C2D-C1D-CHD	-2.97	119.37	124.28
2	B	900	HDD	CMC-C2C-C3C	2.97	130.24	124.68
2	C	900	HDD	CMB-C2B-C3B	2.93	130.16	124.68
2	C	900	HDD	O1D-CGD-O2D	2.92	123.41	120.80
2	A	900	HDD	C4C-CHD-C1D	-2.80	124.57	130.12
2	A	900	HDD	CMC-C2C-C3C	2.80	129.91	124.68
2	A	900	HDD	CMB-C2B-C3B	2.77	129.87	124.68
2	C	900	HDD	C3C-C4C-NC	2.75	112.76	109.21
2	D	900	HDD	CMC-C2C-C3C	2.63	129.60	124.68
2	D	900	HDD	CMB-C2B-C3B	2.55	129.46	124.68
2	D	900	HDD	CMA-C3A-C2A	2.34	129.35	124.94
2	A	900	HDD	OND-C2D-CMD	-2.27	105.41	109.59
2	C	900	HDD	CMC-C2C-C3C	2.23	128.85	124.68
2	D	900	HDD	C4C-CHD-C1D	-2.10	125.95	130.12
2	C	900	HDD	OND-C2D-CMD	-2.09	105.75	109.59
2	B	900	HDD	C4C-CHD-C1D	-2.05	126.05	130.12
2	D	900	HDD	OND-C2D-CMD	-2.05	105.82	109.59
2	C	900	HDD	C1A-CHA-C4D	-2.02	126.12	130.12

There are no chirality outliers.

All (1) torsion outliers are listed below:

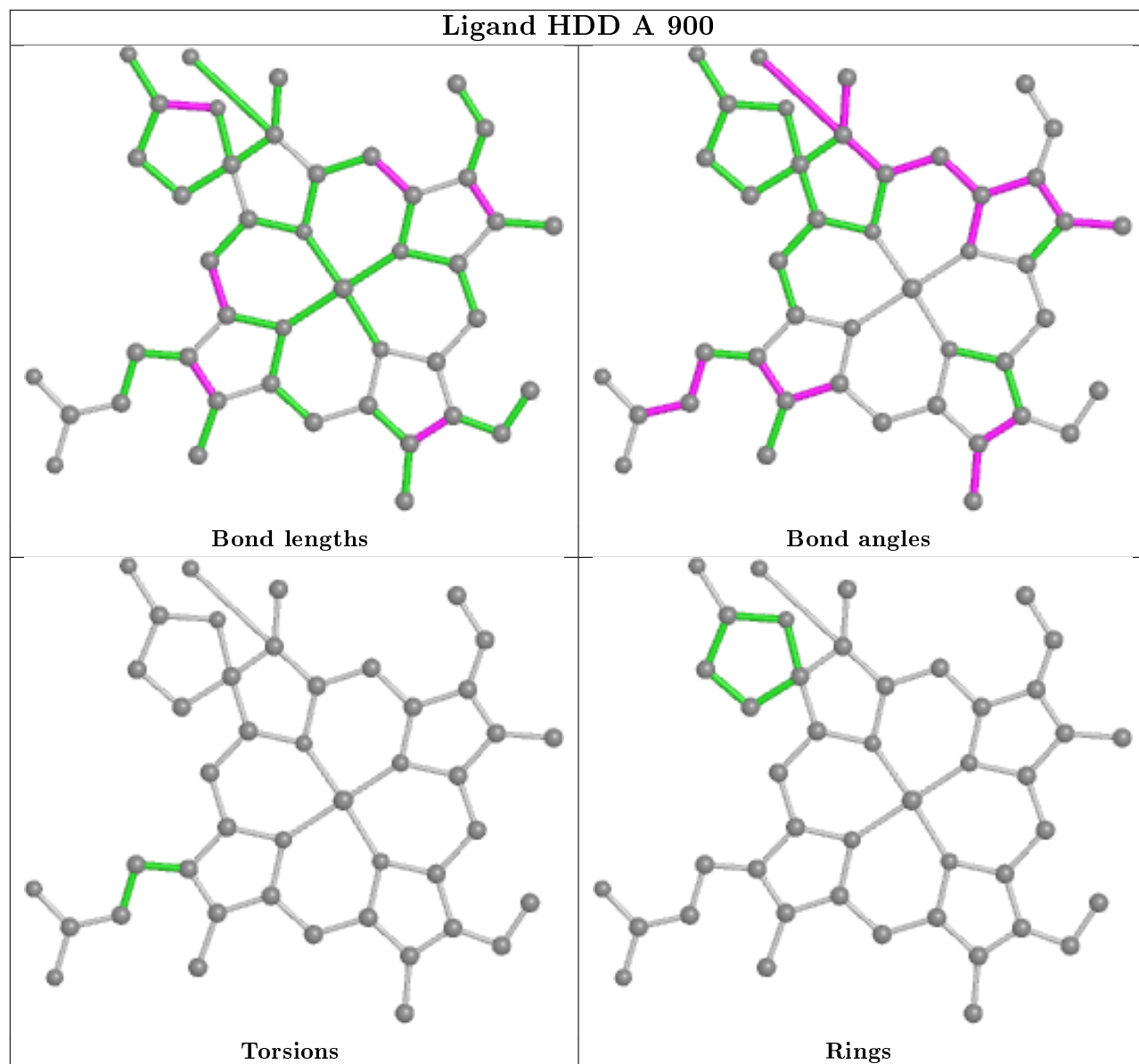
Mol	Chain	Res	Type	Atoms
4	A	1698	1PE	C12-C22-OH3-C23

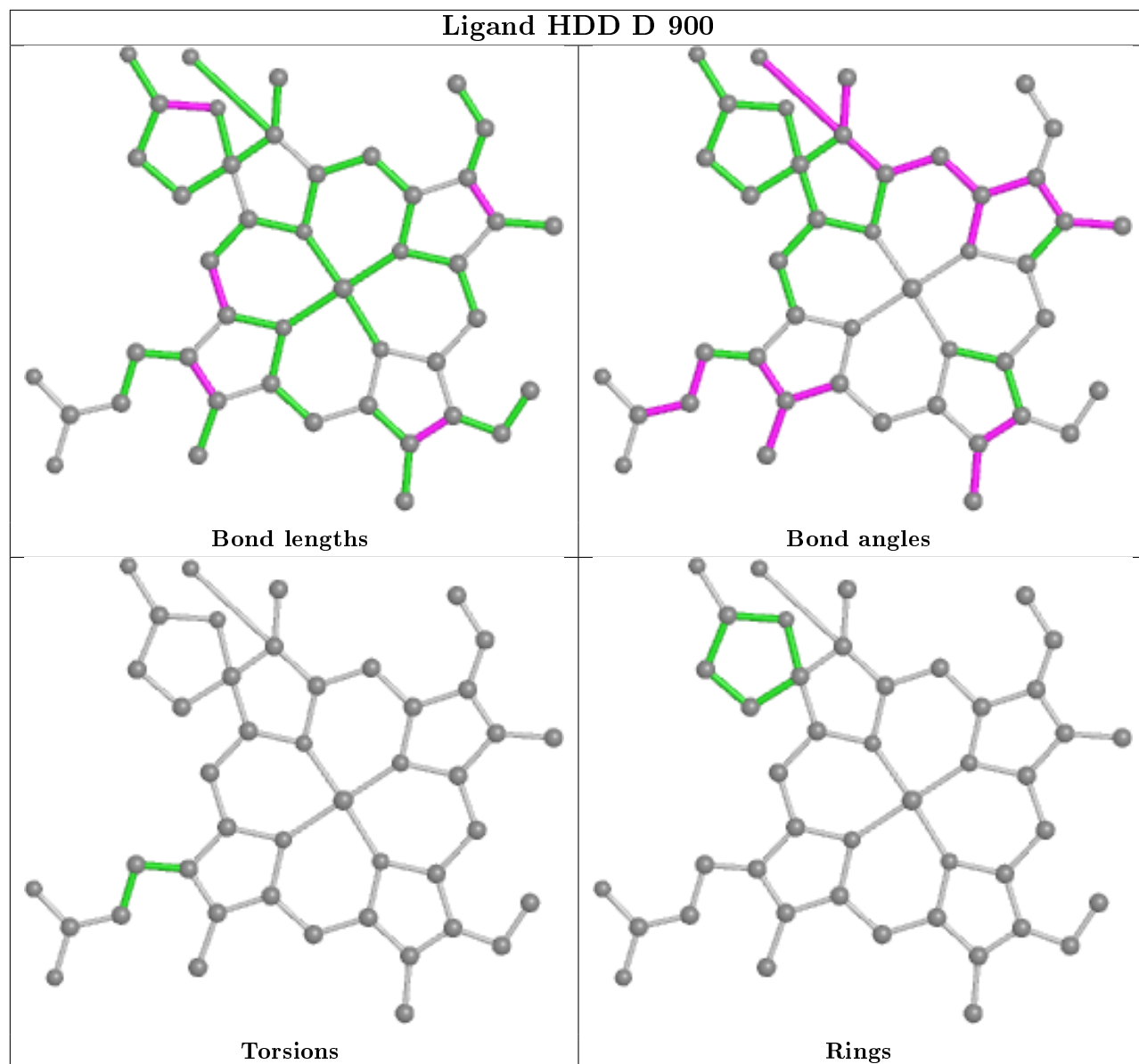
There are no ring outliers.

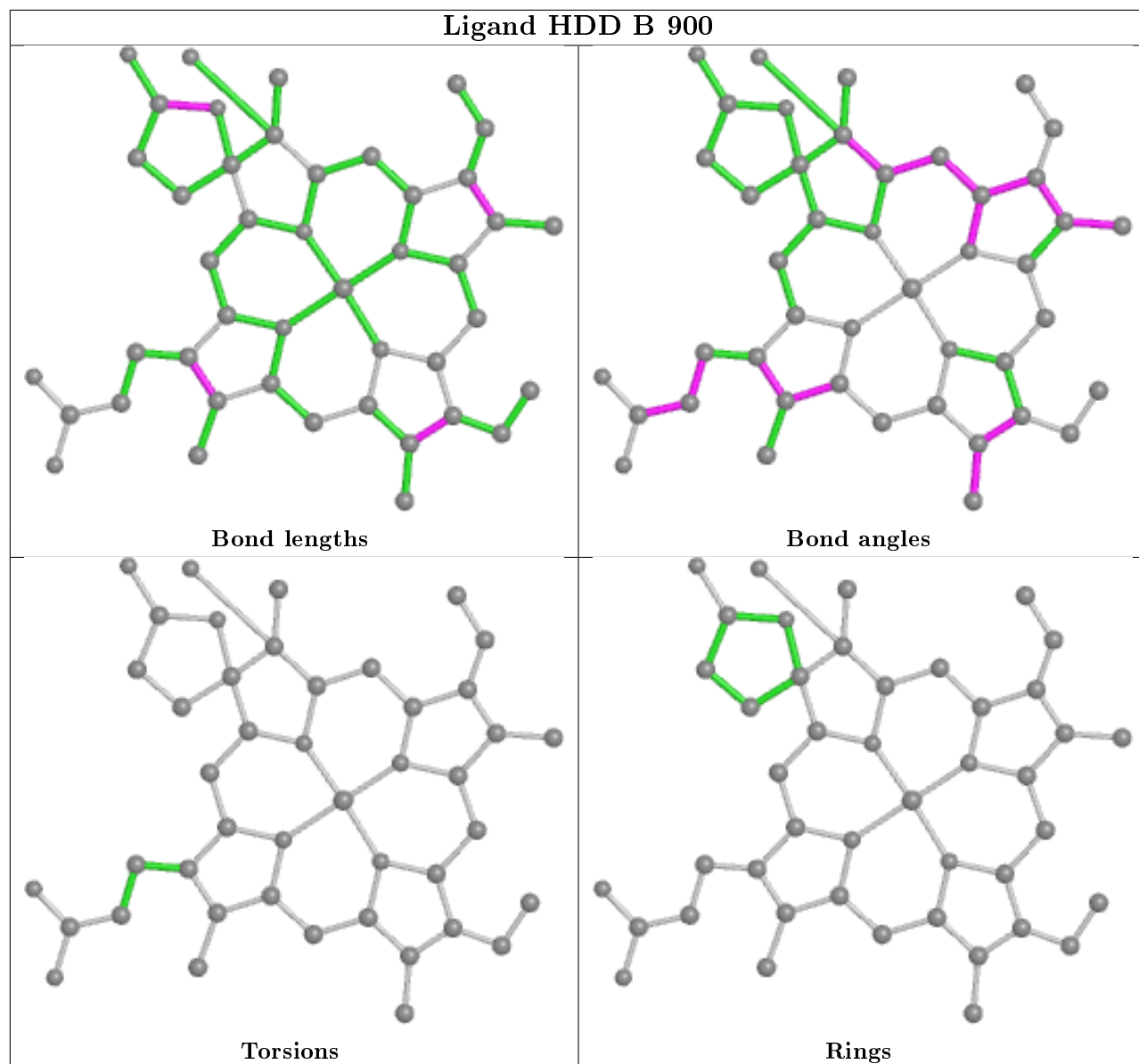
4 monomers are involved in 5 short contacts:

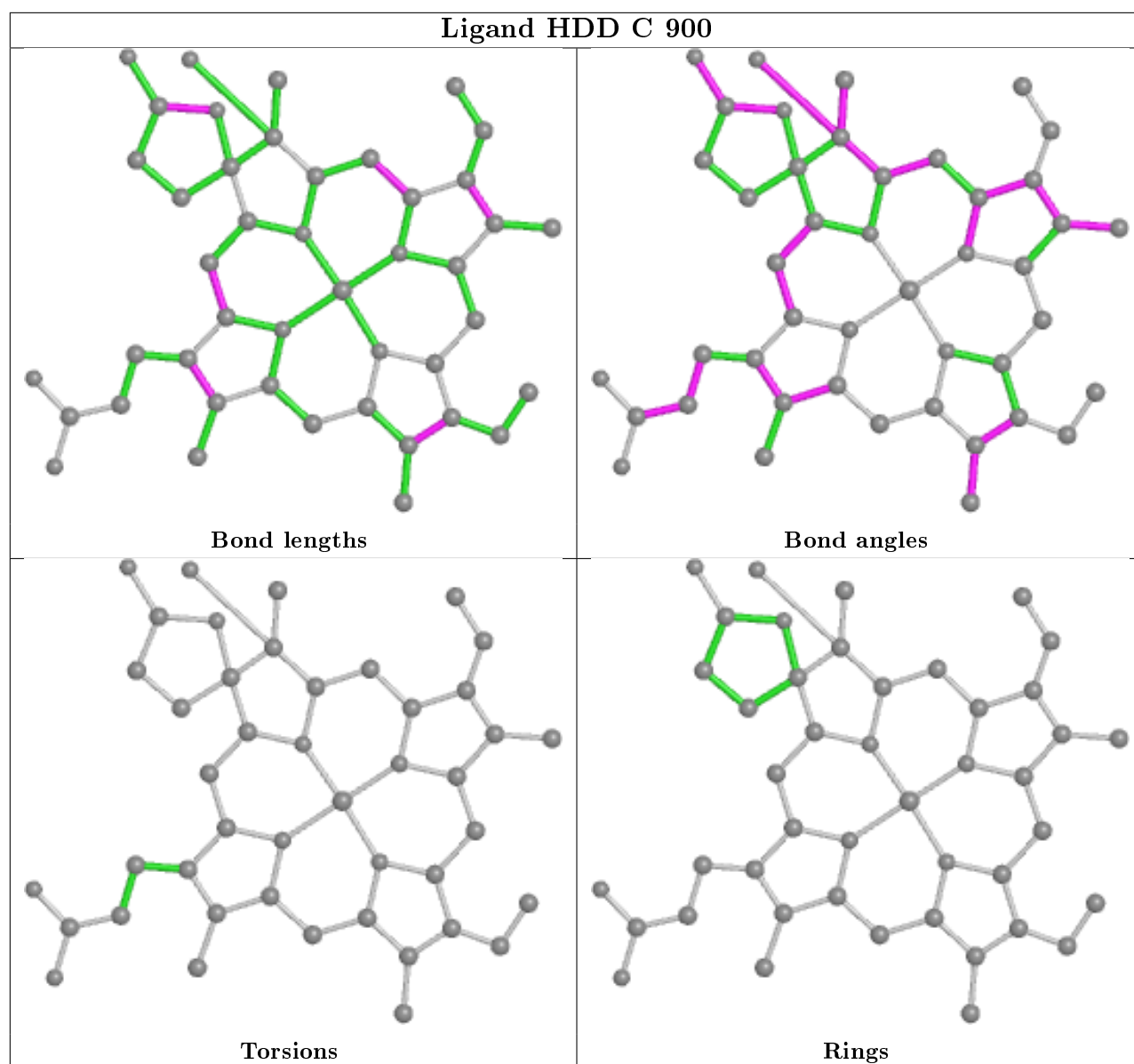
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	HDD	2	0
2	D	900	HDD	1	0
2	B	900	HDD	1	0
2	C	900	HDD	1	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	673/719 (93%)	-0.38	6 (0%) 84 82	5, 10, 21, 35	0
1	B	673/719 (93%)	-0.35	8 (1%) 79 77	6, 12, 24, 36	0
1	C	671/719 (93%)	-0.32	21 (3%) 49 48	5, 11, 28, 66	0
1	D	671/719 (93%)	-0.23	32 (4%) 30 30	5, 12, 34, 67	0
All	All	2688/2876 (93%)	-0.32	67 (2%) 57 57	5, 11, 27, 67	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	672	GLU	6.3
1	D	653	SER	5.8
1	C	672	GLU	5.1
1	D	674	VAL	4.9
1	D	618	ALA	4.7
1	C	618	ALA	4.5
1	D	561	SER	4.3
1	D	611	ASP	4.1
1	D	22	PRO	4.0
1	D	649	GLY	3.9
1	C	653	SER	3.7
1	C	22	PRO	3.7
1	C	676[A]	MET	3.6
1	C	673	SER	3.6
1	D	590[A]	GLU	3.6
1	D	673	SER	3.5
1	D	658	ALA	3.5
1	D	671	GLU	3.5
1	B	576[A]	LYS	3.4
1	C	318	TYR	3.4
1	A	22	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	676[A]	MET	3.3
1	D	657	ASP	3.1
1	B	664	ASP	3.1
1	B	517	GLY	3.0
1	C	674	VAL	3.0
1	C	561	SER	3.0
1	D	576	LYS	3.0
1	C	611	ASP	3.0
1	A	318	TYR	2.9
1	C	671	GLU	2.9
1	C	560	GLU	2.8
1	D	660	ASP	2.8
1	C	590[A]	GLU	2.8
1	A	622	SER	2.8
1	D	565	ASP	2.7
1	A	561	SER	2.6
1	D	572	THR	2.6
1	D	648	CYS	2.5
1	D	675	ASP	2.5
1	D	560	GLU	2.5
1	D	562	SER	2.5
1	C	657	ASP	2.5
1	D	664	ASP	2.5
1	B	318	TYR	2.5
1	B	622	SER	2.5
1	D	659	ALA	2.4
1	C	21	SER	2.4
1	D	564	LEU	2.4
1	D	21	SER	2.3
1	C	660	ASP	2.3
1	D	23	LEU	2.3
1	A	430	ASN	2.3
1	B	698	SER	2.2
1	D	318	TYR	2.2
1	C	559[A]	SER	2.2
1	D	655	VAL	2.2
1	D	615	ALA	2.1
1	D	302	ALA	2.1
1	B	590[A]	GLU	2.1
1	C	573[A]	ARG	2.1
1	C	614	ALA	2.1
1	A	21	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	657	ASP	2.0
1	C	675	ASP	2.0
1	C	649	GLY	2.0
1	D	654	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

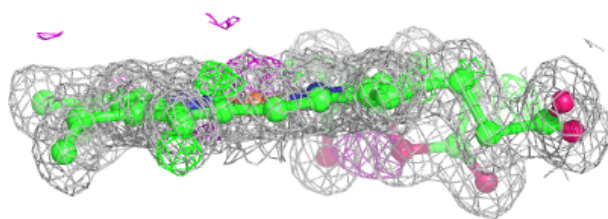
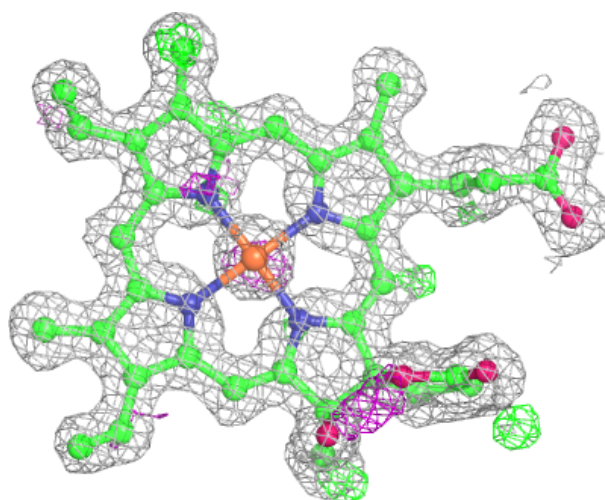
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	1PE	A	1698	16/16	0.76	0.20	9,11,13,15	16
2	HDD	C	900	44/44	0.98	0.08	5,6,9,13	0
2	HDD	A	900	44/44	0.98	0.07	5,7,9,13	0
2	HDD	D	900	44/44	0.98	0.08	5,7,10,14	0
2	HDD	B	900	44/44	0.98	0.07	6,7,10,13	0
3	CA	C	1699	1/1	1.00	0.10	13,13,13,13	1
3	CA	A	910	1/1	1.00	0.04	11,11,11,11	1
3	CA	C	1698	1/1	1.00	0.08	7,7,7,7	1
3	CA	B	1701	1/1	1.00	0.07	13,13,13,13	1
3	CA	A	1700	1/1	1.00	0.08	12,12,12,12	1
3	CA	B	1699	1/1	1.00	0.07	9,9,9,9	1
3	CA	D	1699	1/1	1.00	0.08	17,17,17,17	1
3	CA	A	1699	1/1	1.00	0.03	9,9,9,9	1
3	CA	B	1700	1/1	1.00	0.04	15,15,15,15	1
3	CA	D	1698	1/1	1.00	0.05	11,11,11,11	1

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.

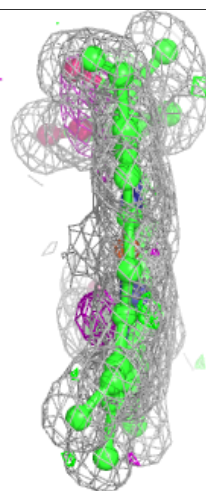
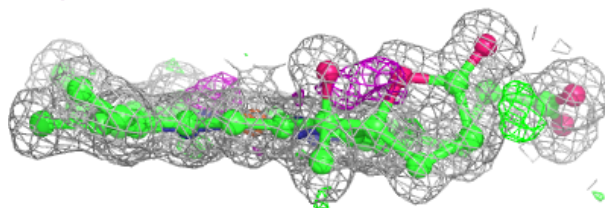
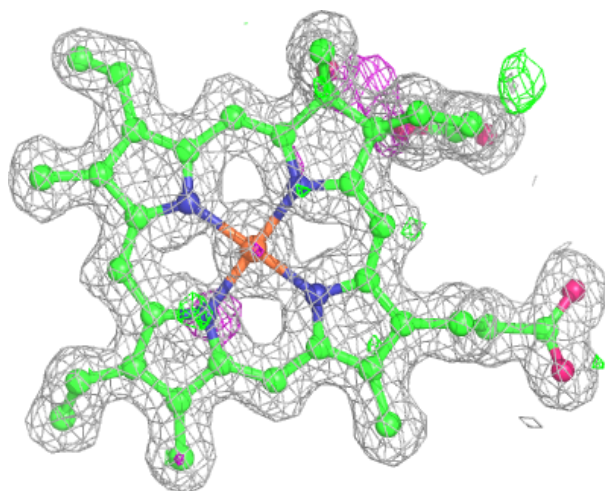
**Electron density around HDD C 900:**

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



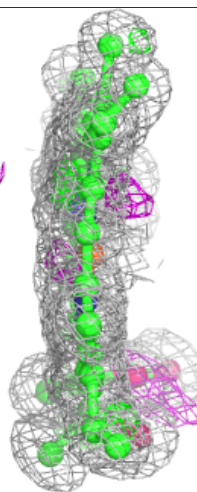
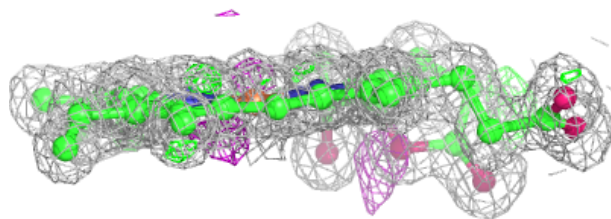
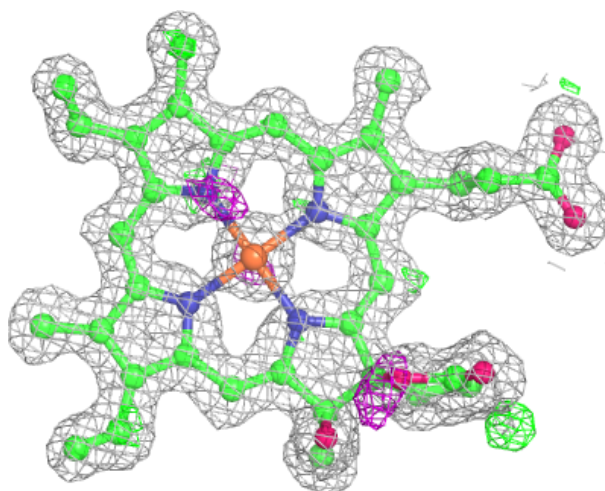
**Electron density around HDD A 900:**

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



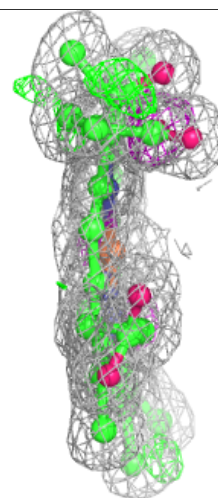
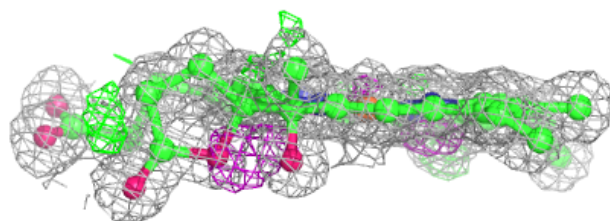
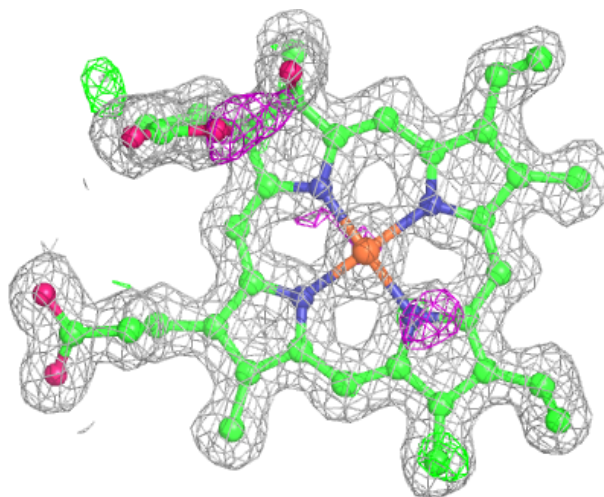
**Electron density around HDD D 900:**

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



**Electron density around HDD B 900:**

$2mF_o-DF_c$  (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.