



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:10 PM UTC

PDB ID : 7RTQ / pdb_00007rtq
Title : Sterol 14alpha demethylase (CYP51) from Naegleria fowleri in complex with an inhibitor R)-N-(1-(3,4'-difluorobiphenyl-4-yl)-2-(1H-imidazol-1-yl)ethyl)-4-(5-phenyl-1,3,4-oxadiazol-2-yl)benzamide
Authors : Lepesheva, G.I.; Hargrove, T.Y.; Wawrzak, Z.
Deposited on : 2021-08-13
Resolution : 2.11 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

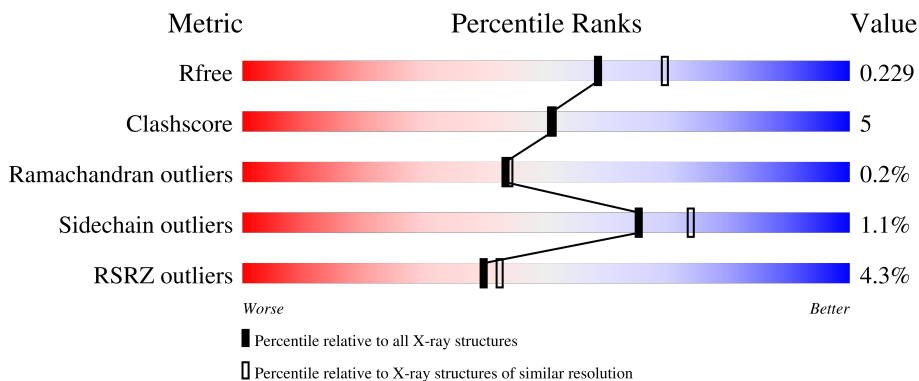
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

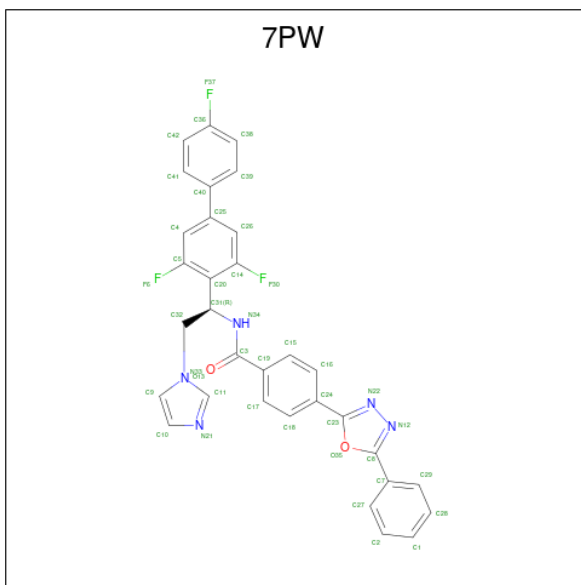
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. 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	466	
1	B	466	
1	C	466	
1	D	466	

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

- Molecule 3 is N-[(1R)-2-(1H-imidazol-1-yl)-1-(3,4',5-trifluoro[1,1'-biphenyl]-4-yl)ethyl]-4-(5-phenyl-1,3,4-oxadiazol-2-yl)benzamide (CCD ID: 7PW) (formula: C₃₂H₂₂F₃N₅O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total	C	F	N	O	0	1
			84	64	6	10	4		
3	B	1	Total	C	F	N	O	0	1
			84	64	6	10	4		
3	C	1	Total	C	F	N	O	0	1
			84	64	6	10	4		
3	D	1	Total	C	F	N	O	0	1
			84	64	6	10	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	214	Total	O	0	0
			214	214		
4	B	249	Total	O	0	0
			249	249		

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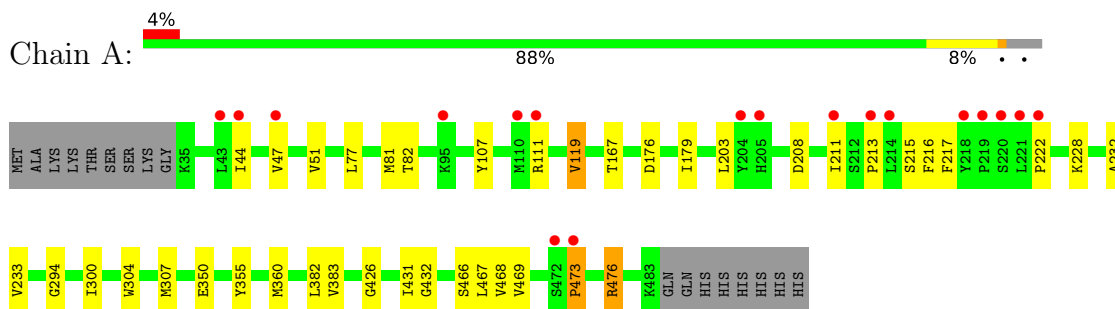
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	245	Total 245	O 245	0	0
4	D	233	Total 233	O 233	0	0

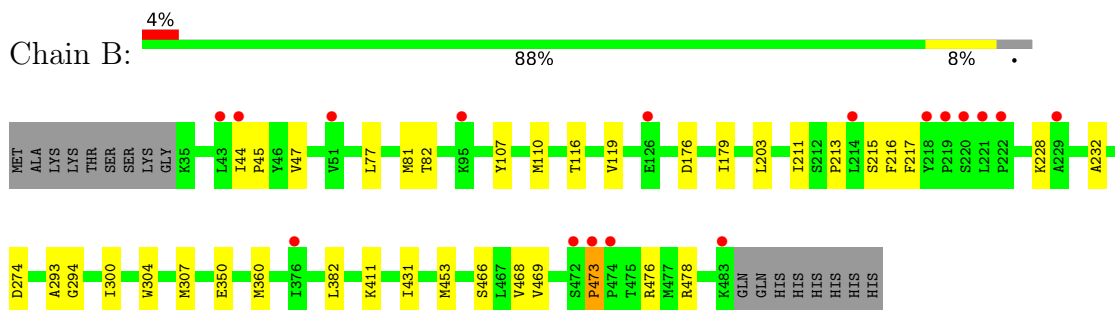
3 Residue-property plots [i](#)

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.

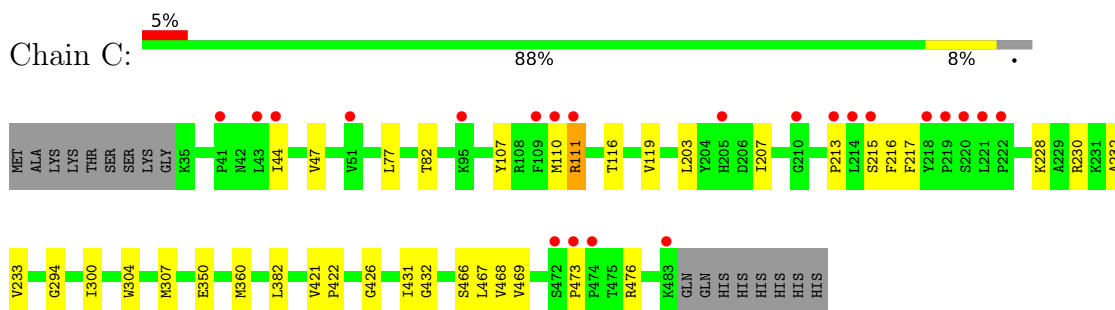
- Molecule 1: Protein CYP51



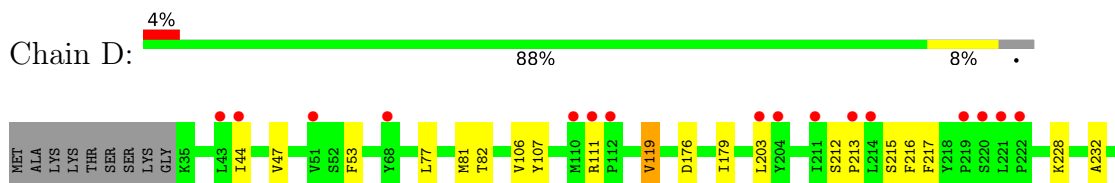
- Molecule 1: Protein CYP51



- Molecule 1: Protein CYP51



- Molecule 1: Protein CYP51





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.06Å 75.22Å 105.95Å 89.49° 74.63° 63.98°	Depositor
Resolution (Å)	64.63 – 2.11 64.63 – 2.11	Depositor EDS
% Data completeness (in resolution range)	96.8 (64.63-2.11) 93.9 (64.63-2.11)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.211 , 0.237 (Not available) , 0.229	Depositor DCC
R_{free} test set	5529 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	21.4	Xtrriage
Anisotropy	0.159	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15917	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 7PW, HEM

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	1.02	0/3695	1.37	6/4981 (0.1%)
1	B	1.02	0/3695	1.38	2/4981 (0.0%)
1	C	1.03	0/3695	1.36	5/4981 (0.1%)
1	D	1.02	0/3695	1.38	3/4981 (0.1%)
All	All	1.02	0/14780	1.38	16/19924 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	473	PRO	N-CA-C	11.15	124.31	110.70
1	A	473	PRO	N-CA-C	10.84	123.92	110.70
1	D	473	PRO	N-CA-C	8.94	121.60	110.70
1	C	473	PRO	N-CA-C	8.85	121.49	110.70
1	A	426	GLY	CA-C-N	5.75	128.30	120.54
1	A	426	GLY	C-N-CA	5.75	128.30	120.54
1	C	426	GLY	CA-C-N	5.72	128.27	120.54
1	C	426	GLY	C-N-CA	5.72	128.27	120.54
1	D	426	GLY	CA-C-N	5.57	128.06	120.54
1	D	426	GLY	C-N-CA	5.57	128.06	120.54
1	B	473	PRO	N-CA-CB	-5.31	97.93	103.08
1	A	208	ASP	CA-CB-CG	5.14	117.74	112.60
1	C	233	VAL	CA-C-N	5.08	125.72	119.99
1	C	233	VAL	C-N-CA	5.08	125.72	119.99
1	A	233	VAL	CA-C-N	5.04	125.69	119.99
1	A	233	VAL	C-N-CA	5.04	125.69	119.99

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	3617	0	3680	37	0
1	B	3617	0	3680	40	0
1	C	3617	0	3680	38	0
1	D	3617	0	3680	39	0
2	A	43	0	30	3	0
2	B	43	0	30	1	0
2	C	43	0	30	2	0
2	D	43	0	30	2	0
3	A	84	0	0	18	0
3	B	84	0	0	17	0
3	C	84	0	0	18	0
3	D	84	0	0	14	0
4	A	214	0	0	3	0
4	B	249	0	0	5	0
4	C	245	0	0	4	0
4	D	233	0	0	3	0
All	All	15917	0	14840	155	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 5.

All (155) 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:D:107:TYR:CE1	3:D:502[A]:7PW:N22	2.40	0.90
1:C:213:PRO:O	3:C:502[A]:7PW:C1	2.19	0.89
1:B:217:PHE:CE1	3:B:502[A]:7PW:C2	2.60	0.84
1:D:360:MET:SD	1:D:383:VAL:HG11	2.19	0.82
1:B:217:PHE:HE1	3:B:502[A]:7PW:C2	1.93	0.81
1:C:111:ARG:NH1	3:C:502[B]:7PW:C1	2.45	0.79
1:D:294:GLY:HA2	2:D:501:HEM:HMC2	1.66	0.77
1:D:213:PRO:O	3:D:502[A]:7PW:C28	2.33	0.77
1:B:360:MET:HE3	3:B:502[A]:7PW:C28	2.15	0.76
1:A:217:PHE:CE1	3:A:502[A]:7PW:C2	2.70	0.75
1:A:213:PRO:O	3:A:502[A]:7PW:C28	2.35	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:GLY:HA2	2:B:501:HEM:HMC2	1.69	0.74
1:D:107:TYR:HE1	3:D:502[A]:7PW:N22	1.85	0.74
1:B:360:MET:CE	3:B:502[A]:7PW:C28	2.66	0.73
1:B:213:PRO:O	3:B:502[A]:7PW:C28	2.37	0.73
1:A:467:LEU:HD11	3:A:502[A]:7PW:C18	2.20	0.72
1:B:107:TYR:HE1	3:B:502[A]:7PW:N22	1.89	0.70
1:A:51:VAL:HG22	4:A:634:HOH:O	1.92	0.69
1:D:217:PHE:CE1	3:D:502[A]:7PW:C2	2.76	0.69
1:C:360:MET:CE	3:C:502[A]:7PW:C28	2.71	0.68
1:B:213:PRO:O	3:B:502[A]:7PW:C1	2.42	0.68
1:B:360:MET:HE1	3:B:502[A]:7PW:C1	2.26	0.66
1:C:213:PRO:O	3:C:502[A]:7PW:C28	2.43	0.66
1:C:360:MET:HE3	3:C:502[A]:7PW:C28	2.26	0.66
1:C:467:LEU:HD11	3:C:502[A]:7PW:C24	2.28	0.64
1:B:411:LYS:NZ	4:B:605:HOH:O	2.29	0.63
1:D:215:SER:OG	3:D:502[B]:7PW:C2	2.47	0.63
1:D:217:PHE:HE1	3:D:502[A]:7PW:C1	2.12	0.62
1:A:217:PHE:HE1	3:A:502[A]:7PW:C2	2.13	0.61
1:A:304:TRP:HA	1:A:307:MET:HE3	1.83	0.61
1:A:217:PHE:HE1	3:A:502[A]:7PW:C1	2.13	0.60
1:C:213:PRO:HB2	3:C:502[A]:7PW:C28	2.32	0.60
1:A:467:LEU:HD11	3:A:502[A]:7PW:C24	2.32	0.60
1:A:294:GLY:HA2	2:A:501:HEM:HMC2	1.84	0.60
1:B:81:MET:HE1	1:B:216:PHE:HE2	1.67	0.60
1:C:213:PRO:O	3:C:502[A]:7PW:C2	2.50	0.60
1:C:304:TRP:HA	1:C:307:MET:HE3	1.84	0.60
1:A:360:MET:CE	3:A:502[A]:7PW:C1	2.80	0.59
1:A:213:PRO:O	3:A:502[A]:7PW:C1	2.51	0.59
1:D:304:TRP:HA	1:D:307:MET:HE3	1.85	0.59
1:A:213:PRO:HD3	1:A:466:SER:O	2.03	0.59
1:C:360:MET:HE1	3:C:502[A]:7PW:C28	2.33	0.58
1:B:304:TRP:HA	1:B:307:MET:HE3	1.84	0.58
1:B:213:PRO:HD3	1:B:466:SER:O	2.03	0.58
1:C:111:ARG:HE	1:C:111:ARG:H	1.52	0.58
1:C:217:PHE:CE1	3:C:502[A]:7PW:C2	2.86	0.58
1:D:81:MET:HE1	1:D:216:PHE:HE2	1.69	0.57
1:D:213:PRO:HD3	1:D:466:SER:O	2.03	0.57
1:B:107:TYR:CE1	3:B:502[A]:7PW:N22	2.70	0.57
1:B:213:PRO:HB2	3:B:502[A]:7PW:C28	2.35	0.57
1:C:213:PRO:HD3	1:C:466:SER:O	2.04	0.57
1:B:360:MET:HE1	3:B:502[A]:7PW:C28	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ILE:HG22	1:A:47:VAL:HG22	1.87	0.56
1:C:44:ILE:HG22	1:C:47:VAL:HG22	1.88	0.56
1:A:81:MET:HE1	1:A:216:PHE:HE2	1.70	0.55
1:D:44:ILE:HG22	1:D:47:VAL:HG22	1.88	0.55
1:D:216:PHE:CD2	3:D:502[A]:7PW:C27	2.90	0.55
1:C:230:ARG:HG2	4:C:768:HOH:O	2.07	0.54
1:D:53:PHE:HZ	1:D:360:MET:HE1	1.73	0.54
1:D:360:MET:SD	1:D:383:VAL:CG1	2.94	0.54
1:A:360:MET:HE1	3:A:502[A]:7PW:C1	2.38	0.54
1:A:222:PRO:HA	4:A:700:HOH:O	2.07	0.53
1:C:47:VAL:HA	1:C:77:LEU:HD23	1.90	0.53
1:D:47:VAL:HA	1:D:77:LEU:HD23	1.90	0.53
1:B:47:VAL:HA	1:B:77:LEU:HD23	1.89	0.53
1:B:293:ALA:HA	4:B:603:HOH:O	2.09	0.53
1:D:106:VAL:HG12	1:D:107:TYR:CE1	2.44	0.53
1:A:47:VAL:HA	1:A:77:LEU:HD23	1.90	0.52
1:B:215:SER:OG	3:B:502[B]:7PW:C2	2.58	0.52
1:C:216:PHE:CB	3:C:502[A]:7PW:C27	2.87	0.51
1:B:110:MET:HB2	4:B:817:HOH:O	2.09	0.51
1:C:432:GLY:HA3	2:C:501:HEM:C3C	2.44	0.51
1:D:107:TYR:CZ	3:D:502[A]:7PW:N22	2.78	0.51
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.93	0.51
1:D:119:VAL:HG22	3:D:502[B]:7PW:C38	2.41	0.51
1:D:360:MET:CE	3:D:502[A]:7PW:C1	2.89	0.51
1:C:116:THR:HG21	4:C:830:HOH:O	2.11	0.51
1:C:110:MET:SD	3:C:502[B]:7PW:O35	2.69	0.50
1:A:360:MET:HE2	3:A:502[A]:7PW:C28	2.42	0.50
1:D:217:PHE:CE1	3:D:502[A]:7PW:C1	2.94	0.50
1:B:116:THR:HG23	4:B:772:HOH:O	2.12	0.49
1:A:215:SER:OG	3:A:502[B]:7PW:C2	2.61	0.49
1:A:360:MET:SD	1:A:383:VAL:HG11	2.52	0.49
1:B:211:ILE:HD12	3:B:502[B]:7PW:C29	2.43	0.49
1:D:106:VAL:HG12	1:D:107:TYR:CD1	2.48	0.49
1:D:106:VAL:HG11	1:D:362:MET:HE3	1.93	0.49
1:A:107:TYR:HE1	3:A:502[A]:7PW:N22	2.11	0.48
1:B:360:MET:CE	3:B:502[A]:7PW:C1	2.91	0.48
1:A:211:ILE:HD12	3:A:502[B]:7PW:C29	2.43	0.48
1:C:116:THR:CG2	4:C:830:HOH:O	2.60	0.48
1:B:217:PHE:HE1	3:B:502[A]:7PW:C1	2.25	0.47
1:B:44:ILE:HB	1:B:47:VAL:HG22	1.96	0.47
1:C:111:ARG:H	1:C:111:ARG:NE	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:MET:CE	1:B:216:PHE:HE2	2.27	0.47
1:C:116:THR:HG22	4:C:766:HOH:O	2.13	0.47
1:D:119:VAL:HG13	3:D:502[B]:7PW:C39	2.45	0.47
1:C:467:LEU:HD21	3:C:502[B]:7PW:C17	2.45	0.47
1:C:107:TYR:HE1	3:C:502[A]:7PW:N22	2.12	0.47
1:C:213:PRO:CB	3:C:502[A]:7PW:C28	2.93	0.47
1:A:44:ILE:CG2	1:A:47:VAL:HG22	2.45	0.47
2:D:501:HEM:HMB1	2:D:501:HEM:HBB2	1.97	0.46
1:C:350:GLU:OE1	1:C:350:GLU:HA	2.16	0.46
1:C:44:ILE:CG2	1:C:47:VAL:HG22	2.45	0.46
1:A:350:GLU:HA	1:A:350:GLU:OE1	2.16	0.46
1:A:467:LEU:CD1	3:A:502[A]:7PW:C18	2.92	0.45
1:D:350:GLU:HA	1:D:350:GLU:OE1	2.17	0.45
1:B:300:ILE:HD12	1:B:468:VAL:HG12	1.98	0.45
1:D:44:ILE:CG2	1:D:47:VAL:HG22	2.46	0.45
1:A:432:GLY:HA3	2:A:501:HEM:C3C	2.52	0.45
1:B:350:GLU:HA	1:B:350:GLU:OE1	2.17	0.45
1:D:467:LEU:HD21	3:D:502[B]:7PW:C17	2.47	0.45
1:D:81:MET:CE	1:D:216:PHE:HE2	2.28	0.45
1:D:431:ILE:C	1:D:431:ILE:HD12	2.42	0.44
1:B:274:ASP:OD2	4:B:601:HOH:O	2.21	0.44
1:A:300:ILE:HD12	1:A:468:VAL:HG12	2.00	0.44
1:B:431:ILE:C	1:B:431:ILE:HD12	2.42	0.44
1:C:431:ILE:C	1:C:431:ILE:HD12	2.43	0.44
1:D:217:PHE:CZ	3:D:502[A]:7PW:C2	3.01	0.44
1:B:44:ILE:HD11	1:C:44:ILE:HG12	2.00	0.43
1:D:334:ASP:OD2	4:D:601:HOH:O	2.21	0.43
1:B:44:ILE:HB	1:B:47:VAL:CG2	2.47	0.43
1:A:82:THR:O	1:A:382:LEU:HA	2.19	0.43
1:B:82:THR:O	1:B:382:LEU:HA	2.18	0.43
1:D:421:VAL:N	1:D:422:PRO:CD	2.82	0.43
1:C:421:VAL:N	1:C:422:PRO:CD	2.82	0.43
1:D:82:THR:O	1:D:382:LEU:HA	2.19	0.43
1:C:203:LEU:HD22	1:C:232:ALA:CB	2.49	0.43
1:D:300:ILE:HD12	1:D:468:VAL:HG12	2.00	0.43
1:B:203:LEU:HD22	1:B:232:ALA:CB	2.49	0.43
1:C:294:GLY:HA2	2:C:501:HEM:HMC2	2.01	0.43
1:A:355:TYR:OH	4:A:601:HOH:O	2.21	0.42
1:D:106:VAL:CG1	1:D:362:MET:HE3	2.49	0.42
1:A:107:TYR:CE1	3:A:502[A]:7PW:N22	2.87	0.42
1:C:300:ILE:HD12	1:C:468:VAL:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:LEU:HD22	1:D:232:ALA:CB	2.49	0.42
1:B:44:ILE:HG23	1:B:45:PRO:HD2	2.01	0.42
1:C:82:THR:O	1:C:382:LEU:HA	2.19	0.42
1:B:213:PRO:CB	3:B:502[A]:7PW:C28	2.98	0.42
1:B:211:ILE:CD1	3:B:502[B]:7PW:C28	2.97	0.42
1:C:111:ARG:NH1	3:C:502[B]:7PW:C2	2.82	0.42
1:C:215:SER:OG	3:C:502[B]:7PW:C2	2.68	0.42
1:A:203:LEU:HD22	1:A:232:ALA:CB	2.49	0.42
1:A:431:ILE:HD12	1:A:431:ILE:C	2.45	0.41
1:B:453:MET:HA	1:B:478:ARG:O	2.21	0.41
1:D:410:ARG:O	4:D:602:HOH:O	2.21	0.41
1:A:119:VAL:HG22	3:A:502[A]:7PW:C38	2.51	0.41
1:A:119:VAL:HG13	3:A:502[A]:7PW:C39	2.51	0.41
1:A:167:THR:OG1	1:A:476:ARG:NH1	2.54	0.41
1:B:107:TYR:O	1:B:110:MET:HB3	2.21	0.41
1:C:360:MET:HE1	3:C:502[A]:7PW:C1	2.51	0.41
1:A:176:ASP:O	1:A:179:ILE:HG22	2.22	0.40
1:B:176:ASP:O	1:B:179:ILE:HG22	2.21	0.40
1:D:410:ARG:HB3	4:D:602:HOH:O	2.21	0.40
1:D:176:ASP:O	1:D:179:ILE:HG22	2.21	0.40
1:A:216:PHE:CB	3:A:502[A]:7PW:C27	2.99	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	447/466 (96%)	435 (97%)	11 (2%)	1 (0%)	43 44
1	B	447/466 (96%)	434 (97%)	12 (3%)	1 (0%)	43 44
1	C	447/466 (96%)	436 (98%)	10 (2%)	1 (0%)	43 44
1	D	447/466 (96%)	435 (97%)	11 (2%)	1 (0%)	43 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1788/1864 (96%)	1740 (97%)	44 (2%)	4 (0%)	43 44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	VAL
1	B	119	VAL
1	C	119	VAL
1	D	119	VAL

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	403/418 (96%)	398 (99%)	5 (1%)	63 71
1	B	403/418 (96%)	399 (99%)	4 (1%)	68 76
1	C	403/418 (96%)	398 (99%)	5 (1%)	63 71
1	D	403/418 (96%)	399 (99%)	4 (1%)	68 76
All	All	1612/1672 (96%)	1594 (99%)	18 (1%)	65 74

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	ARG
1	A	228	LYS
1	A	469	VAL
1	A	473	PRO
1	A	476	ARG
1	B	228	LYS
1	B	469	VAL
1	B	473	PRO
1	B	476	ARG
1	C	111	ARG
1	C	207	ILE

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Mol	Chain	Res	Type
1	C	228	LYS
1	C	469	VAL
1	C	476	ARG
1	D	111	ARG
1	D	212	SER
1	D	228	LYS
1	D	469	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	GLN
1	A	276	GLN
1	B	270	GLN
1	B	276	GLN
1	B	308	ASN
1	C	270	GLN
1	C	276	GLN
1	C	308	ASN
1	D	270	GLN
1	D	276	GLN
1	D	308	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	7PW	B	502[A]	2	47,47,47	3.05	8 (17%)	63,66,66	1.95	22 (34%)
3	7PW	A	502[A]	2	47,47,47	3.32	10 (21%)	63,66,66	2.15	26 (41%)
3	7PW	C	502[B]	2	47,47,47	2.88	11 (23%)	63,66,66	1.49	13 (20%)
2	HEM	C	501	3,1	50,50,50	1.62	9 (18%)	67,82,82	1.51	13 (19%)
3	7PW	D	502[A]	2	47,47,47	3.04	9 (19%)	63,66,66	2.11	21 (33%)
2	HEM	B	501	3,1	50,50,50	1.64	8 (16%)	67,82,82	1.50	10 (14%)
2	HEM	A	501	3,1	50,50,50	1.66	9 (18%)	67,82,82	1.53	12 (17%)
2	HEM	D	501	3,1	50,50,50	1.65	7 (14%)	67,82,82	1.53	13 (19%)
3	7PW	B	502[B]	2	47,47,47	2.58	11 (23%)	63,66,66	1.52	16 (25%)
3	7PW	A	502[B]	2	47,47,47	2.69	12 (25%)	63,66,66	1.63	13 (20%)
3	7PW	C	502[A]	2	47,47,47	3.56	10 (21%)	63,66,66	1.99	22 (34%)
3	7PW	D	502[B]	2	47,47,47	2.67	11 (23%)	63,66,66	1.60	13 (20%)

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	7PW	B	502[A]	2	-	4/28/28/28	0/6/6/6
3	7PW	A	502[A]	2	-	5/28/28/28	0/6/6/6
3	7PW	C	502[B]	2	-	4/28/28/28	0/6/6/6
2	HEM	C	501	3,1	-	3/14/54/54	-
3	7PW	D	502[A]	2	-	3/28/28/28	0/6/6/6
2	HEM	B	501	3,1	-	3/14/54/54	-
2	HEM	A	501	3,1	-	0/14/54/54	-
2	HEM	D	501	3,1	-	0/14/54/54	-
3	7PW	B	502[B]	2	-	3/28/28/28	0/6/6/6
3	7PW	A	502[B]	2	-	5/28/28/28	0/6/6/6
3	7PW	C	502[A]	2	-	5/28/28/28	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	7PW	D	502[B]	2	-	2/28/28/28	0/6/6/6

All (115) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502[A]	7PW	C20-C31	-11.64	1.40	1.52
3	D	502[A]	7PW	C20-C31	-10.99	1.41	1.52
3	A	502[A]	7PW	C20-C31	-10.92	1.41	1.52
3	B	502[A]	7PW	C20-C31	-10.83	1.41	1.52
3	C	502[A]	7PW	O35-C8	-10.18	1.21	1.37
3	A	502[A]	7PW	O35-C23	-10.11	1.21	1.37
3	A	502[B]	7PW	C20-C31	-10.05	1.42	1.52
3	C	502[A]	7PW	F30-C14	-9.94	1.08	1.35
3	C	502[B]	7PW	C20-C31	-9.90	1.42	1.52
3	D	502[B]	7PW	C20-C31	-9.65	1.42	1.52
3	C	502[B]	7PW	F30-C14	-9.26	1.10	1.35
3	B	502[B]	7PW	C20-C31	-8.86	1.43	1.52
3	D	502[A]	7PW	C24-C23	-8.35	1.30	1.47
3	C	502[A]	7PW	C7-C8	-8.35	1.30	1.47
3	B	502[A]	7PW	C7-C8	-8.29	1.30	1.47
3	D	502[A]	7PW	C7-C8	-8.16	1.30	1.47
3	A	502[A]	7PW	C24-C23	-8.08	1.31	1.47
3	B	502[A]	7PW	C24-C23	-8.04	1.31	1.47
3	C	502[A]	7PW	C24-C23	-7.97	1.31	1.47
3	A	502[A]	7PW	C7-C8	-7.79	1.31	1.47
3	B	502[A]	7PW	O35-C8	-7.72	1.24	1.37
3	A	502[A]	7PW	O35-C8	-7.41	1.25	1.37
3	C	502[B]	7PW	C7-C8	-7.20	1.32	1.47
3	D	502[B]	7PW	C7-C8	-7.07	1.33	1.47
3	B	502[B]	7PW	C7-C8	-6.88	1.33	1.47
3	D	502[A]	7PW	O35-C8	-6.83	1.26	1.37
3	D	502[B]	7PW	C24-C23	-6.58	1.34	1.47
3	B	502[B]	7PW	O35-C8	-6.57	1.26	1.37
3	B	502[B]	7PW	C24-C23	-6.53	1.34	1.47
3	D	502[B]	7PW	O35-C8	-6.33	1.27	1.37
3	A	502[B]	7PW	C7-C8	-6.21	1.34	1.47
3	B	502[A]	7PW	O35-C23	-6.20	1.27	1.37
3	A	502[B]	7PW	C24-C23	-6.18	1.34	1.47
3	C	502[B]	7PW	C24-C23	-6.09	1.35	1.47
3	D	502[A]	7PW	O35-C23	-6.05	1.27	1.37
3	C	502[A]	7PW	C19-C3	-5.93	1.37	1.50
3	A	502[B]	7PW	C8-N12	5.92	1.38	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502[A]	7PW	C19-C3	-5.87	1.37	1.50
3	D	502[A]	7PW	C19-C3	-5.86	1.37	1.50
3	A	502[B]	7PW	C23-N22	5.61	1.37	1.29
3	B	502[A]	7PW	C19-C3	-5.55	1.38	1.50
2	C	501	HEM	FE-NB	5.48	2.11	1.94
2	B	501	HEM	FE-NB	5.43	2.11	1.94
2	D	501	HEM	FE-NB	5.36	2.11	1.94
2	A	501	HEM	FE-NB	5.34	2.11	1.94
3	C	502[A]	7PW	O35-C23	-5.18	1.29	1.37
3	C	502[B]	7PW	C23-N22	4.69	1.36	1.29
2	D	501	HEM	FE-NC	4.51	2.10	1.95
3	A	502[B]	7PW	F6-C5	-4.42	1.23	1.35
2	A	501	HEM	FE-NC	4.37	2.09	1.95
3	B	502[B]	7PW	C19-C3	-4.31	1.40	1.50
2	B	501	HEM	FE-NC	4.30	2.09	1.95
3	D	502[B]	7PW	C23-N22	4.21	1.35	1.29
2	C	501	HEM	FE-NC	4.12	2.08	1.95
2	D	501	HEM	C1B-NB	-4.08	1.33	1.40
2	A	501	HEM	C1B-NB	-4.06	1.33	1.40
3	C	502[A]	7PW	C25-C40	-4.02	1.39	1.49
3	B	502[A]	7PW	C25-C40	-4.01	1.39	1.49
3	A	502[B]	7PW	C25-C40	-4.00	1.39	1.49
3	D	502[A]	7PW	C25-C40	-4.00	1.39	1.49
3	A	502[B]	7PW	C19-C3	-3.99	1.41	1.50
3	C	502[B]	7PW	C25-C40	-3.92	1.39	1.49
3	A	502[A]	7PW	F6-C5	-3.92	1.25	1.35
3	A	502[A]	7PW	C25-C40	-3.92	1.39	1.49
3	C	502[A]	7PW	N12-N22	-3.86	1.31	1.39
2	B	501	HEM	C1B-NB	-3.84	1.33	1.40
3	C	502[B]	7PW	C19-C3	-3.82	1.41	1.50
3	D	502[B]	7PW	C19-C3	-3.80	1.41	1.50
2	C	501	HEM	C1B-NB	-3.77	1.33	1.40
3	D	502[B]	7PW	C8-N12	3.76	1.35	1.29
3	D	502[B]	7PW	C25-C40	-3.74	1.40	1.49
3	B	502[A]	7PW	N12-N22	-3.73	1.31	1.39
3	A	502[A]	7PW	N12-N22	-3.65	1.31	1.39
3	B	502[B]	7PW	C25-C40	-3.62	1.40	1.49
3	C	502[B]	7PW	O35-C8	-3.61	1.31	1.37
3	B	502[B]	7PW	O35-C23	-3.61	1.31	1.37
3	C	502[B]	7PW	C8-N12	3.59	1.34	1.29
2	A	501	HEM	C4D-ND	-3.55	1.34	1.40
3	D	502[A]	7PW	N12-N22	-3.53	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	C4D-ND	-3.45	1.34	1.40
3	A	502[A]	7PW	F37-C36	3.43	1.44	1.36
2	C	501	HEM	C4D-ND	-3.40	1.34	1.40
2	B	501	HEM	C4D-ND	-3.19	1.34	1.40
3	B	502[B]	7PW	C23-N22	3.13	1.34	1.29
3	D	502[B]	7PW	O35-C23	-3.12	1.32	1.37
3	B	502[B]	7PW	N12-N22	-2.96	1.33	1.39
3	D	502[B]	7PW	F30-C14	-2.89	1.27	1.35
3	B	502[B]	7PW	C8-N12	2.67	1.33	1.29
3	D	502[B]	7PW	N12-N22	-2.67	1.34	1.39
2	B	501	HEM	C1C-C2C	-2.64	1.40	1.45
2	D	501	HEM	C1C-C2C	-2.57	1.40	1.45
2	A	501	HEM	C4B-NB	-2.57	1.33	1.38
3	B	502[B]	7PW	C31-N34	2.56	1.49	1.46
2	C	501	HEM	C1C-C2C	-2.50	1.40	1.45
2	B	501	HEM	C4B-NB	-2.48	1.34	1.38
3	A	502[B]	7PW	F37-C36	2.46	1.42	1.36
3	D	502[A]	7PW	F30-C14	-2.45	1.29	1.35
2	D	501	HEM	C4B-NB	-2.45	1.34	1.38
2	A	501	HEM	C1C-C2C	-2.41	1.40	1.45
3	A	502[B]	7PW	N12-N22	-2.41	1.34	1.39
3	C	502[B]	7PW	N12-N22	-2.36	1.34	1.39
2	D	501	HEM	C1D-ND	-2.34	1.34	1.38
2	B	501	HEM	C1D-ND	-2.30	1.34	1.38
2	A	501	HEM	C1D-ND	-2.25	1.34	1.38
2	B	501	HEM	FE-ND	-2.22	1.88	1.94
2	C	501	HEM	C4B-NB	-2.20	1.34	1.38
3	C	502[B]	7PW	C20-C5	2.18	1.41	1.39
3	C	502[A]	7PW	C8-N12	2.16	1.32	1.29
2	C	501	HEM	C1D-ND	-2.13	1.34	1.38
2	A	501	HEM	C1A-C2A	-2.11	1.40	1.44
2	A	501	HEM	FE-ND	-2.08	1.88	1.94
2	C	501	HEM	C3C-C4C	-2.07	1.42	1.46
3	A	502[B]	7PW	C31-N34	2.07	1.49	1.46
2	C	501	HEM	FE-ND	-2.04	1.88	1.94
3	A	502[B]	7PW	O35-C23	-2.01	1.34	1.37

All (194) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502[A]	7PW	C31-N34-C3	-5.17	116.19	122.34
3	C	502[A]	7PW	C31-N34-C3	-5.13	116.23	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	CHC-C4B-NB	4.93	129.73	124.42
2	C	501	HEM	CHC-C4B-NB	4.90	129.70	124.42
2	A	501	HEM	CHC-C4B-NB	4.75	129.53	124.42
2	B	501	HEM	CHC-C4B-NB	4.62	129.40	124.42
3	D	502[A]	7PW	C16-C24-C18	4.50	124.29	118.57
3	A	502[A]	7PW	C16-C24-C18	4.22	123.93	118.57
3	B	502[A]	7PW	C7-C8-N12	-4.21	121.82	128.36
3	C	502[B]	7PW	O35-C23-N22	-4.20	108.55	112.34
3	C	502[A]	7PW	C7-C8-N12	-4.19	121.86	128.36
3	B	502[B]	7PW	C8-O35-C23	4.10	106.60	102.64
3	A	502[A]	7PW	C24-C23-N22	-4.10	121.99	128.36
3	D	502[A]	7PW	C32-C31-N34	-4.08	100.29	110.71
3	D	502[A]	7PW	C7-C8-N12	-4.06	122.05	128.36
3	A	502[B]	7PW	C31-N34-C3	-4.04	117.53	122.34
2	D	501	HEM	CHD-C1D-ND	3.98	128.71	124.42
3	D	502[A]	7PW	C31-N34-C3	-3.94	117.65	122.34
3	D	502[A]	7PW	C17-C18-C24	-3.94	116.59	120.80
3	D	502[A]	7PW	C5-C20-C14	3.92	119.26	114.27
3	A	502[A]	7PW	C17-C18-C24	-3.90	116.63	120.80
3	C	502[A]	7PW	C32-C31-N34	-3.88	100.80	110.71
3	A	502[A]	7PW	C32-C31-N34	-3.88	100.81	110.71
3	D	502[A]	7PW	C24-C23-N22	-3.84	122.40	128.36
3	D	502[B]	7PW	C32-N33-C11	-3.83	121.58	126.96
3	D	502[B]	7PW	C31-N34-C3	-3.82	117.80	122.34
2	B	501	HEM	CHD-C1D-ND	3.80	128.52	124.42
3	B	502[A]	7PW	C31-N34-C3	-3.79	117.83	122.34
2	C	501	HEM	CHD-C1D-ND	3.78	128.49	124.42
3	A	502[A]	7PW	C15-C19-C17	3.76	123.35	118.57
3	A	502[A]	7PW	C7-C8-N12	-3.75	122.54	128.36
3	A	502[A]	7PW	C16-C15-C19	-3.73	116.81	120.80
3	C	502[A]	7PW	C24-C23-N22	-3.70	122.61	128.36
3	C	502[A]	7PW	C15-C19-C17	3.63	123.19	118.57
3	D	502[B]	7PW	C8-O35-C23	3.61	106.13	102.64
3	C	502[A]	7PW	C16-C24-C18	3.57	123.11	118.57
3	D	502[A]	7PW	C16-C15-C19	-3.55	117.01	120.80
3	B	502[A]	7PW	C32-C31-N34	-3.54	101.68	110.71
3	B	502[B]	7PW	C31-N34-C3	-3.53	118.14	122.34
3	A	502[A]	7PW	C8-N12-N22	-3.52	102.99	106.33
2	A	501	HEM	CHD-C1D-ND	3.52	128.21	124.42
3	D	502[A]	7PW	C15-C19-C17	3.51	123.03	118.57
3	A	502[B]	7PW	C32-N33-C11	-3.49	122.06	126.96
3	D	502[A]	7PW	C28-C29-C7	-3.47	116.96	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502[A]	7PW	C5-C20-C14	3.45	118.67	114.27
3	B	502[A]	7PW	C16-C24-C18	3.43	122.93	118.57
3	C	502[B]	7PW	C31-N34-C3	-3.36	118.34	122.34
3	B	502[A]	7PW	C24-C23-N22	-3.35	123.15	128.36
3	C	502[A]	7PW	C5-C20-C14	3.29	118.45	114.27
3	C	502[A]	7PW	C16-C15-C19	-3.27	117.31	120.80
3	A	502[B]	7PW	C25-C4-C5	3.19	122.13	119.61
3	C	502[B]	7PW	C8-O35-C23	3.19	105.72	102.64
3	C	502[A]	7PW	F6-C5-C20	3.17	121.96	118.14
3	B	502[A]	7PW	C29-C7-C27	3.17	122.59	118.57
3	D	502[A]	7PW	C29-C7-C27	3.14	122.56	118.57
3	B	502[A]	7PW	C16-C15-C19	-3.11	117.48	120.80
2	B	501	HEM	CHA-C4D-ND	3.11	128.21	124.37
3	A	502[A]	7PW	O35-C8-C7	3.07	124.08	118.73
3	B	502[A]	7PW	C17-C18-C24	-3.06	117.53	120.80
2	A	501	HEM	C1B-NB-C4B	3.05	108.82	105.21
3	A	502[B]	7PW	C19-C3-N34	3.05	122.69	117.04
3	B	502[B]	7PW	O35-C23-N22	-3.05	109.59	112.34
3	C	502[A]	7PW	O35-C23-C24	3.04	124.02	118.73
2	C	501	HEM	CHA-C4D-ND	3.01	128.09	124.37
3	C	502[B]	7PW	F6-C5-C20	3.00	121.75	118.14
3	A	502[A]	7PW	C4-C25-C40	3.00	125.87	120.84
2	D	501	HEM	C1B-NB-C4B	3.00	108.75	105.21
3	C	502[A]	7PW	C23-N22-N12	-2.98	103.51	106.33
3	D	502[A]	7PW	O13-C3-C19	-2.96	115.03	120.90
3	C	502[B]	7PW	C32-N33-C11	-2.96	122.80	126.96
3	A	502[B]	7PW	O35-C8-C7	2.96	123.89	118.73
3	D	502[B]	7PW	C5-C20-C14	2.96	118.03	114.27
2	A	501	HEM	CHA-C4D-ND	2.94	128.01	124.37
3	C	502[B]	7PW	C25-C4-C5	2.93	121.92	119.61
3	D	502[A]	7PW	O35-C8-C7	2.90	123.79	118.73
3	B	502[A]	7PW	C15-C19-C17	2.90	122.26	118.57
3	A	502[B]	7PW	C25-C26-C14	2.89	121.90	119.61
3	A	502[A]	7PW	O35-C23-C24	2.88	123.74	118.73
3	B	502[B]	7PW	C25-C26-C14	2.87	121.88	119.61
3	A	502[B]	7PW	C8-O35-C23	2.87	105.41	102.64
3	D	502[B]	7PW	O35-C23-N22	-2.86	109.76	112.34
3	D	502[A]	7PW	O35-C23-C24	2.85	123.70	118.73
3	A	502[A]	7PW	C5-C20-C14	2.84	117.89	114.27
3	B	502[A]	7PW	C28-C29-C7	-2.84	117.57	120.36
2	D	501	HEM	CHA-C4D-ND	2.82	127.86	124.37
3	B	502[A]	7PW	O35-C8-C7	2.82	123.64	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	C4B-C3B-C2B	-2.82	104.69	107.28
3	C	502[B]	7PW	C5-C20-C14	2.80	117.84	114.27
2	C	501	HEM	C1B-NB-C4B	2.79	108.52	105.21
2	B	501	HEM	C1B-NB-C4B	2.79	108.51	105.21
2	C	501	HEM	C4B-C3B-C2B	-2.79	104.72	107.28
3	B	502[A]	7PW	O35-C23-C24	2.78	123.57	118.73
2	D	501	HEM	C4B-C3B-C2B	-2.76	104.74	107.28
2	B	501	HEM	CHA-C4D-C3D	-2.76	120.15	125.23
2	D	501	HEM	CHD-C1D-C2D	-2.74	120.70	125.03
2	A	501	HEM	CHA-C4D-C3D	-2.72	120.21	125.23
3	C	502[A]	7PW	O35-C8-C7	2.71	123.46	118.73
2	A	501	HEM	C4B-C3B-C2B	-2.69	104.81	107.28
3	C	502[B]	7PW	O35-C23-C24	2.68	123.40	118.73
3	B	502[B]	7PW	C32-N33-C11	-2.67	123.20	126.96
3	D	502[B]	7PW	C42-C36-C38	-2.67	119.30	122.80
3	C	502[A]	7PW	C17-C18-C24	-2.65	117.97	120.80
3	A	502[B]	7PW	C4-C25-C40	2.63	125.25	120.84
3	A	502[B]	7PW	O35-C23-C24	2.63	123.31	118.73
2	C	501	HEM	CHA-C4D-C3D	-2.63	120.39	125.23
3	D	502[A]	7PW	C17-C19-C3	-2.63	112.09	120.60
3	B	502[A]	7PW	C17-C19-C3	-2.62	112.10	120.60
3	A	502[A]	7PW	C27-C7-C8	-2.62	116.58	120.56
3	B	502[A]	7PW	C8-N12-N22	-2.62	103.85	106.33
3	B	502[B]	7PW	C19-C3-N34	2.60	121.86	117.04
3	A	502[A]	7PW	C8-O35-C23	2.59	105.14	102.64
3	C	502[A]	7PW	O35-C8-N12	2.59	114.68	112.34
3	D	502[B]	7PW	C25-C4-C5	2.57	121.64	119.61
3	C	502[A]	7PW	C4-C5-C20	-2.55	120.13	124.43
3	B	502[B]	7PW	O35-C8-C7	2.55	123.17	118.73
2	C	501	HEM	CHD-C1D-C2D	-2.54	121.02	125.03
3	B	502[B]	7PW	O35-C23-C24	2.54	123.15	118.73
3	B	502[A]	7PW	C26-C14-C20	-2.54	120.15	124.43
3	A	502[A]	7PW	C29-C7-C27	2.52	121.78	118.57
2	A	501	HEM	CHD-C1D-C2D	-2.52	121.05	125.03
3	C	502[A]	7PW	C29-C7-C27	2.51	121.77	118.57
2	D	501	HEM	CHA-C4D-C3D	-2.51	120.61	125.23
3	B	502[A]	7PW	F6-C5-C20	2.51	121.15	118.14
3	C	502[A]	7PW	C17-C19-C3	-2.48	112.57	120.60
3	C	502[B]	7PW	F30-C14-C20	2.47	121.11	118.14
3	A	502[A]	7PW	C26-C25-C40	-2.47	116.70	120.84
2	B	501	HEM	CHD-C1D-C2D	-2.46	121.15	125.03
2	C	501	HEM	CHD-C4C-NC	2.46	127.13	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502[B]	7PW	O13-C3-N34	-2.44	117.82	122.47
3	B	502[B]	7PW	C5-C20-C14	2.44	117.37	114.27
3	D	502[A]	7PW	C32-N33-C11	-2.43	123.55	126.96
3	B	502[A]	7PW	O35-C8-N12	2.43	114.53	112.34
3	A	502[B]	7PW	C5-C20-C14	2.42	117.35	114.27
2	A	501	HEM	O2A-CGA-CBA	2.41	121.61	114.00
3	A	502[A]	7PW	C32-N33-C11	-2.40	123.58	126.96
3	A	502[A]	7PW	C42-C36-C38	-2.40	119.65	122.80
2	B	501	HEM	CHB-C1B-NB	2.39	127.32	124.37
3	A	502[A]	7PW	C25-C26-C14	2.38	121.49	119.61
3	B	502[A]	7PW	C27-C7-C8	-2.38	116.96	120.56
3	C	502[B]	7PW	C25-C26-C14	2.38	121.49	119.61
2	D	501	HEM	O2A-CGA-CBA	2.38	121.51	114.00
2	A	501	HEM	CHB-C1B-NB	2.36	127.29	124.37
2	C	501	HEM	C1A-CHA-C4D	-2.32	120.78	126.25
3	C	502[A]	7PW	C27-C7-C8	-2.31	117.06	120.56
3	D	502[A]	7PW	C4-C5-C20	-2.30	120.55	124.43
3	B	502[B]	7PW	C26-C14-C20	-2.30	120.56	124.43
3	A	502[B]	7PW	O35-C23-N22	-2.28	110.28	112.34
2	C	501	HEM	CHA-C1A-NA	2.26	127.96	123.86
3	D	502[B]	7PW	C4-C25-C40	2.26	124.62	120.84
3	B	502[B]	7PW	F6-C5-C20	2.26	120.86	118.14
3	D	502[A]	7PW	C18-C24-C23	-2.25	117.14	120.56
3	A	502[A]	7PW	C25-C4-C5	2.25	121.39	119.61
3	C	502[B]	7PW	C7-C8-N12	-2.25	124.86	128.36
2	D	501	HEM	CHB-C1B-NB	2.24	127.14	124.37
3	C	502[B]	7PW	C4-C5-C20	-2.24	120.65	124.43
3	A	502[A]	7PW	C28-C29-C7	-2.23	118.17	120.36
3	C	502[B]	7PW	C26-C14-C20	-2.22	120.69	124.43
3	B	502[A]	7PW	C4-C5-C20	-2.21	120.71	124.43
2	B	501	HEM	O2A-CGA-CBA	2.21	120.97	114.00
3	C	502[A]	7PW	C18-C24-C23	-2.21	117.22	120.56
3	D	502[A]	7PW	C26-C14-C20	-2.20	120.72	124.43
3	A	502[B]	7PW	C18-C17-C19	2.18	123.13	120.80
3	D	502[B]	7PW	O35-C23-C24	2.18	122.53	118.73
3	A	502[A]	7PW	C16-C24-C23	-2.18	117.26	120.56
3	B	502[A]	7PW	F30-C14-C20	2.17	120.75	118.14
3	B	502[B]	7PW	C41-C42-C36	2.16	120.60	118.38
3	D	502[A]	7PW	C42-C36-C38	-2.16	119.97	122.80
2	A	501	HEM	O2D-CGD-CBD	2.14	120.76	114.00
3	A	502[A]	7PW	C17-C19-C3	-2.14	113.67	120.60
2	D	501	HEM	C1A-CHA-C4D	-2.14	121.22	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502[B]	7PW	O13-C3-N34	-2.13	118.41	122.47
3	B	502[B]	7PW	C25-C4-C5	2.13	121.29	119.61
3	B	502[B]	7PW	F30-C14-C20	2.11	120.68	118.14
3	D	502[B]	7PW	C25-C26-C14	2.11	121.27	119.61
3	D	502[B]	7PW	C19-C3-N34	2.10	120.94	117.04
2	A	501	HEM	CHA-C1A-NA	2.10	127.66	123.86
3	C	502[A]	7PW	C32-N33-C11	-2.09	124.03	126.96
3	A	502[A]	7PW	C4-C5-C20	-2.08	120.93	124.43
2	C	501	HEM	O2A-CGA-CBA	2.07	120.55	114.00
3	A	502[B]	7PW	C7-C8-N12	-2.07	125.15	128.36
2	D	501	HEM	O2D-CGD-O1D	-2.06	118.03	123.33
2	C	501	HEM	CHB-C1B-NB	2.06	126.92	124.37
2	A	501	HEM	C1A-CHA-C4D	-2.05	121.43	126.25
3	C	502[A]	7PW	C28-C29-C7	-2.05	118.35	120.36
3	A	502[A]	7PW	C39-C38-C36	2.03	120.47	118.38
3	B	502[B]	7PW	C7-C8-N12	-2.03	125.20	128.36
3	D	502[B]	7PW	C4-C5-C20	-2.03	121.01	124.43
2	B	501	HEM	C1A-CHA-C4D	-2.03	121.48	126.25
2	D	501	HEM	CHA-C1A-NA	2.03	127.53	123.86
2	D	501	HEM	O2D-CGD-CBD	2.02	120.38	114.00
2	C	501	HEM	O2D-CGD-O1D	-2.02	118.14	123.33
3	C	502[A]	7PW	O13-C3-C19	-2.02	116.90	120.90
3	B	502[A]	7PW	O13-C3-C19	-2.01	116.91	120.90
3	D	502[A]	7PW	O35-C8-N12	2.00	114.14	112.34

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	HEM	C2C-C3C-CAC-CBC
3	A	502[A]	7PW	C14-C20-C31-C32
3	A	502[B]	7PW	C14-C20-C31-C32
3	A	502[B]	7PW	C14-C20-C31-N34
3	A	502[B]	7PW	C5-C20-C31-C32
3	A	502[B]	7PW	C5-C20-C31-N34
3	B	502[A]	7PW	C14-C20-C31-C32
3	B	502[A]	7PW	C5-C20-C31-C32
3	B	502[A]	7PW	C20-C31-N34-C3
3	B	502[B]	7PW	C14-C20-C31-C32
3	B	502[B]	7PW	C5-C20-C31-C32
3	B	502[B]	7PW	C5-C20-C31-N34
3	C	502[A]	7PW	C14-C20-C31-C32

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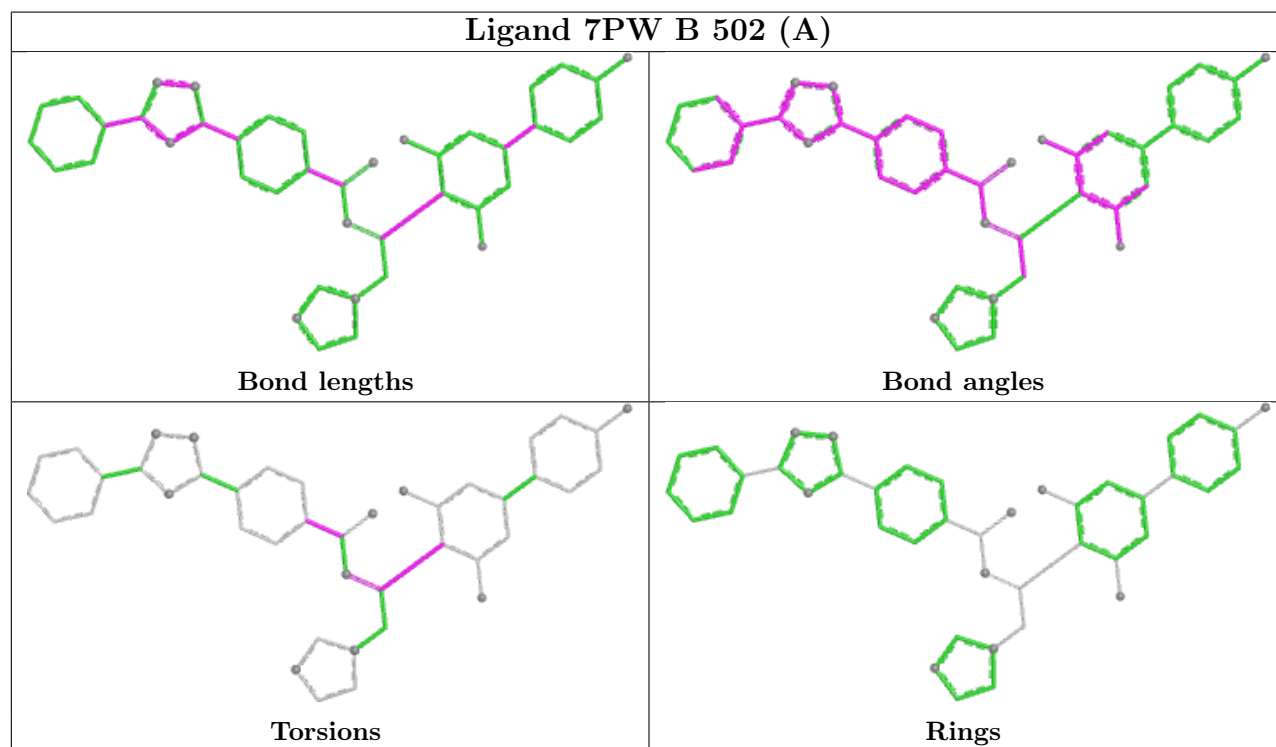
Mol	Chain	Res	Type	Atoms
3	C	502[A]	7PW	C5-C20-C31-C32
3	C	502[A]	7PW	C5-C20-C31-N34
3	C	502[B]	7PW	C14-C20-C31-N34
3	C	502[B]	7PW	C5-C20-C31-C32
3	C	502[B]	7PW	C5-C20-C31-N34
3	D	502[B]	7PW	C14-C20-C31-C32
3	D	502[B]	7PW	C5-C20-C31-C32
3	D	502[A]	7PW	C20-C31-N34-C3
2	C	501	HEM	C4C-C3C-CAC-CBC
3	A	502[A]	7PW	C20-C31-N34-C3
3	C	502[A]	7PW	C20-C31-N34-C3
3	A	502[A]	7PW	C5-C20-C31-C32
3	C	502[B]	7PW	C14-C20-C31-C32
3	D	502[A]	7PW	C5-C20-C31-C32
3	C	502[A]	7PW	C15-C19-C3-N34
3	D	502[A]	7PW	C15-C19-C3-N34
3	A	502[A]	7PW	C15-C19-C3-N34
3	B	502[A]	7PW	C15-C19-C3-N34
3	A	502[B]	7PW	C32-C31-N34-C3
2	B	501	HEM	CAA-CBA-CGA-O1A
3	A	502[A]	7PW	C17-C19-C3-N34
2	B	501	HEM	CAA-CBA-CGA-O2A
2	C	501	HEM	CAA-CBA-CGA-O2A
2	B	501	HEM	C2C-C3C-CAC-CBC

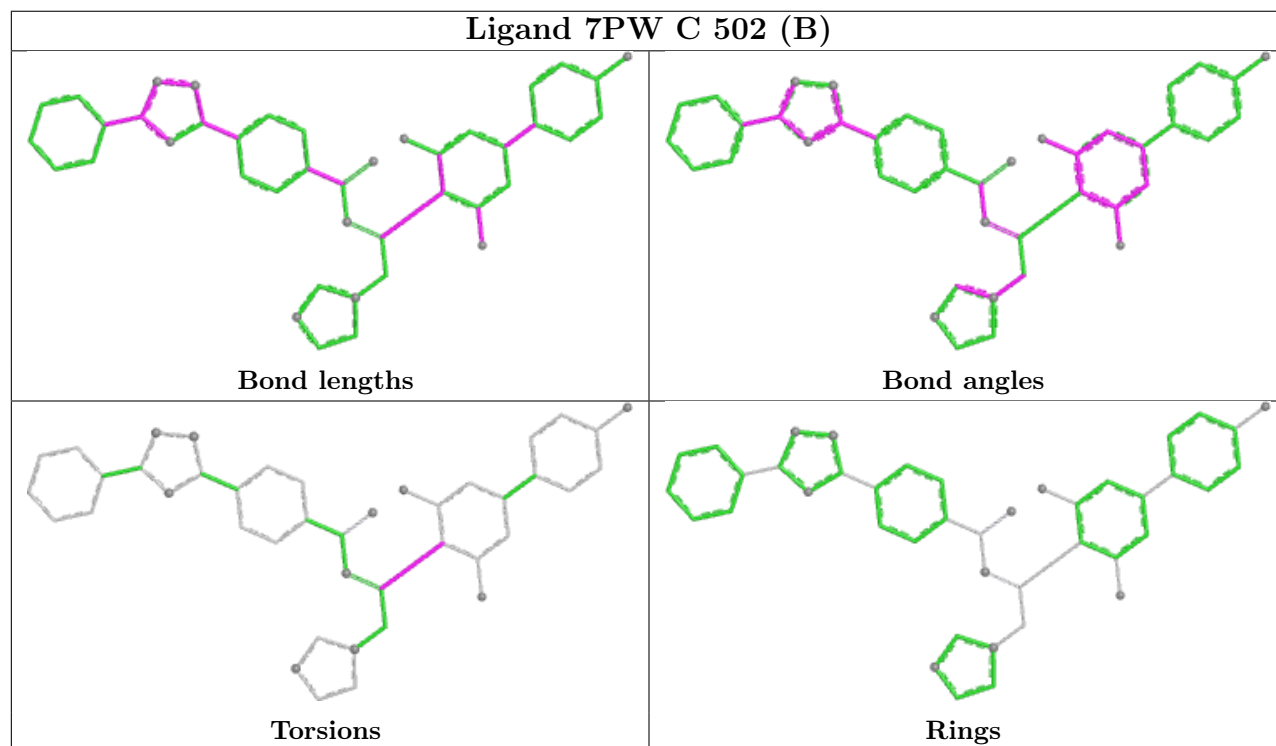
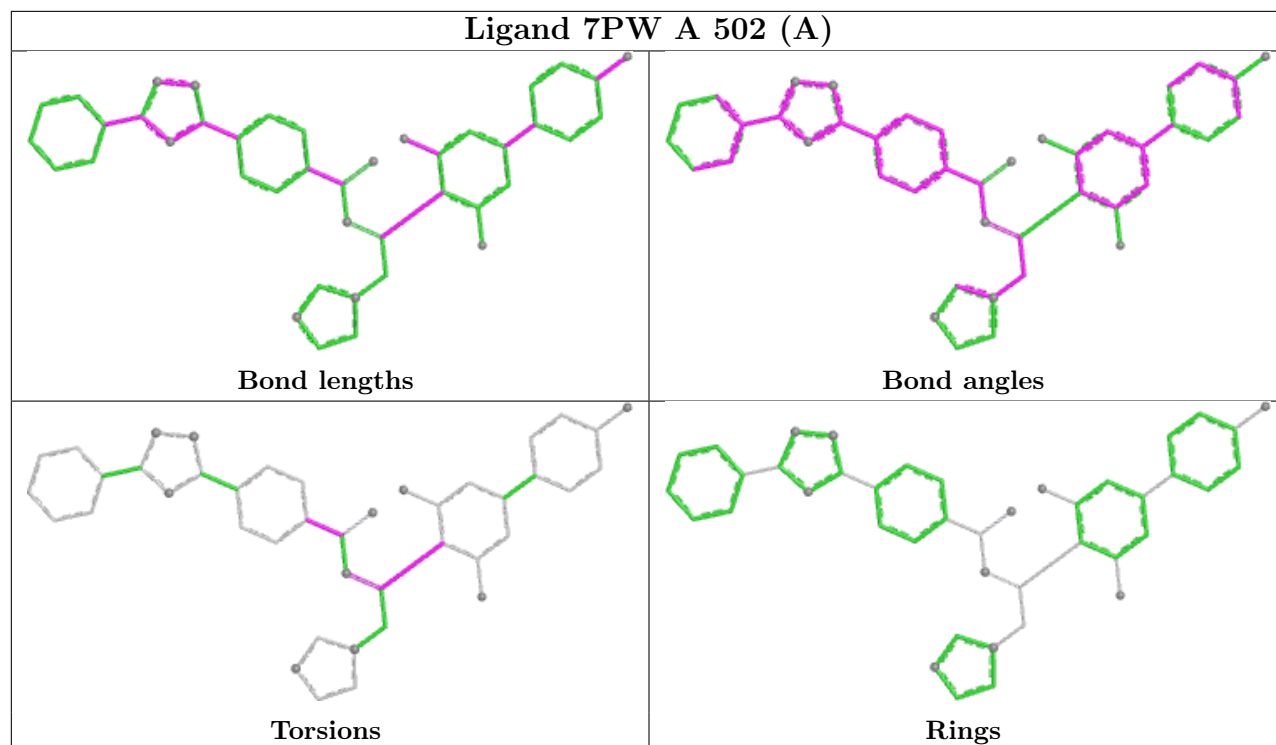
There are no ring outliers.

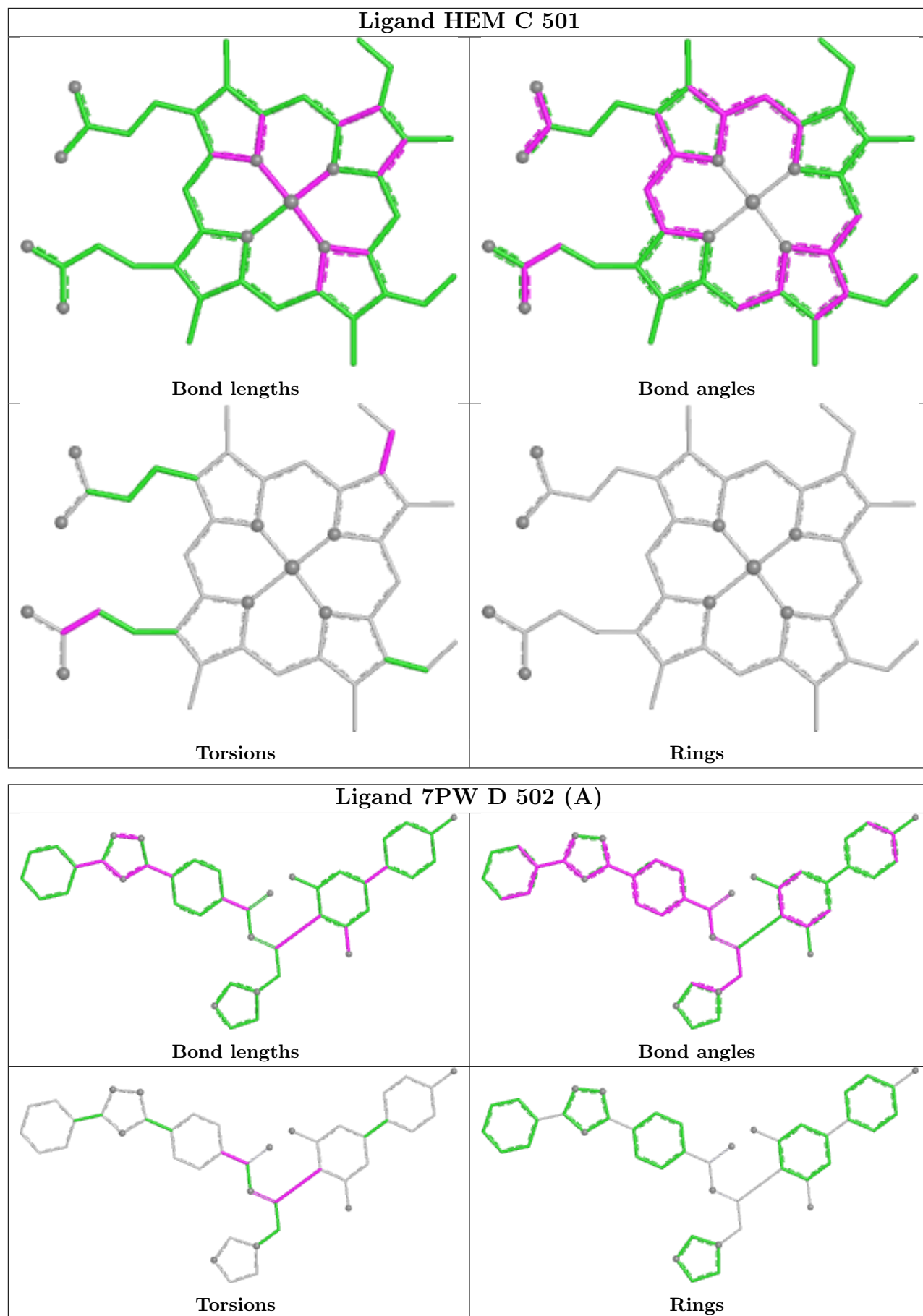
12 monomers are involved in 75 short contacts:

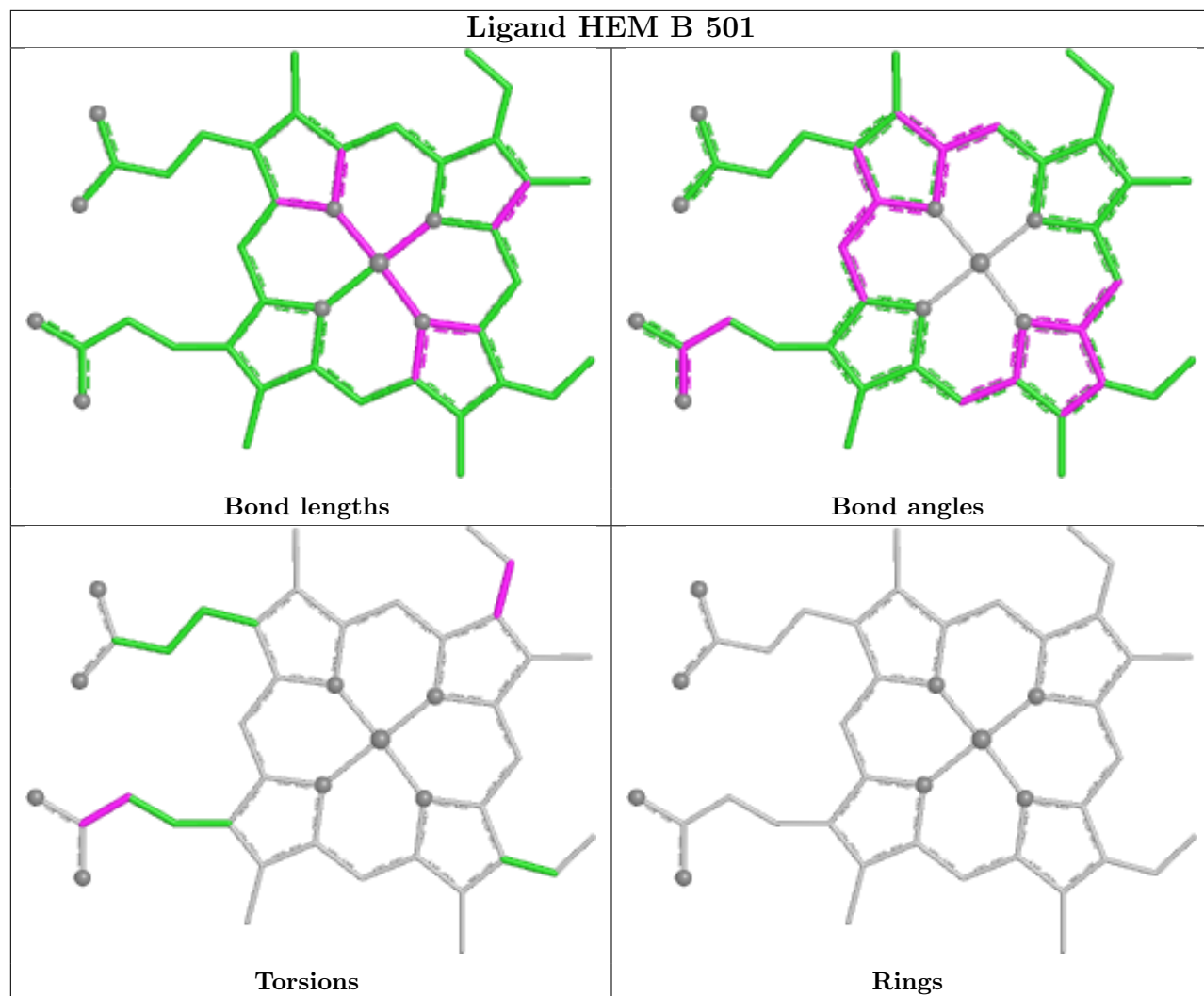
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502[A]	7PW	14	0
3	A	502[A]	7PW	16	0
3	C	502[B]	7PW	5	0
2	C	501	HEM	2	0
3	D	502[A]	7PW	10	0
2	B	501	HEM	1	0
2	A	501	HEM	3	0
2	D	501	HEM	2	0
3	B	502[B]	7PW	3	0
3	A	502[B]	7PW	2	0
3	C	502[A]	7PW	13	0
3	D	502[B]	7PW	4	0

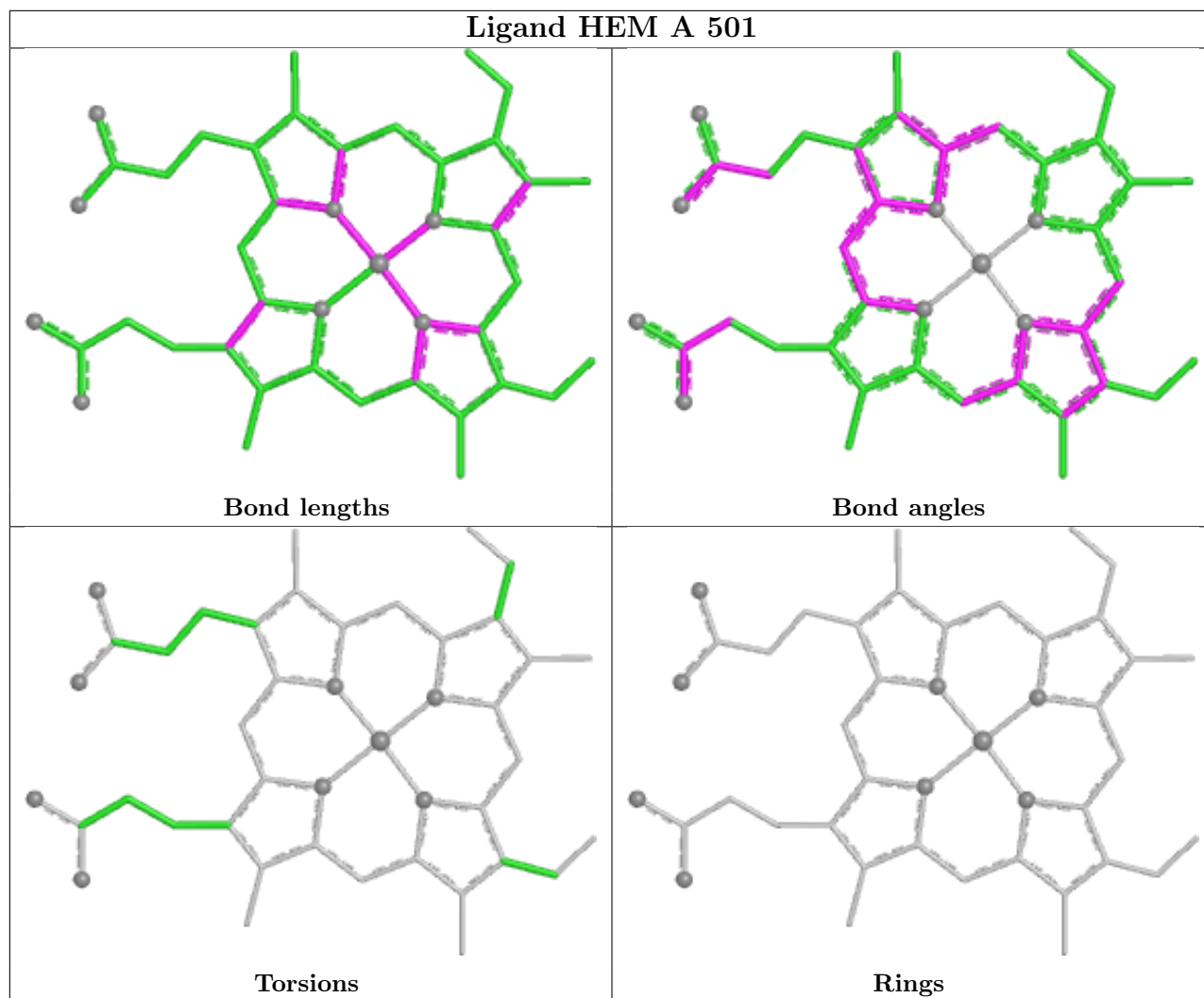
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

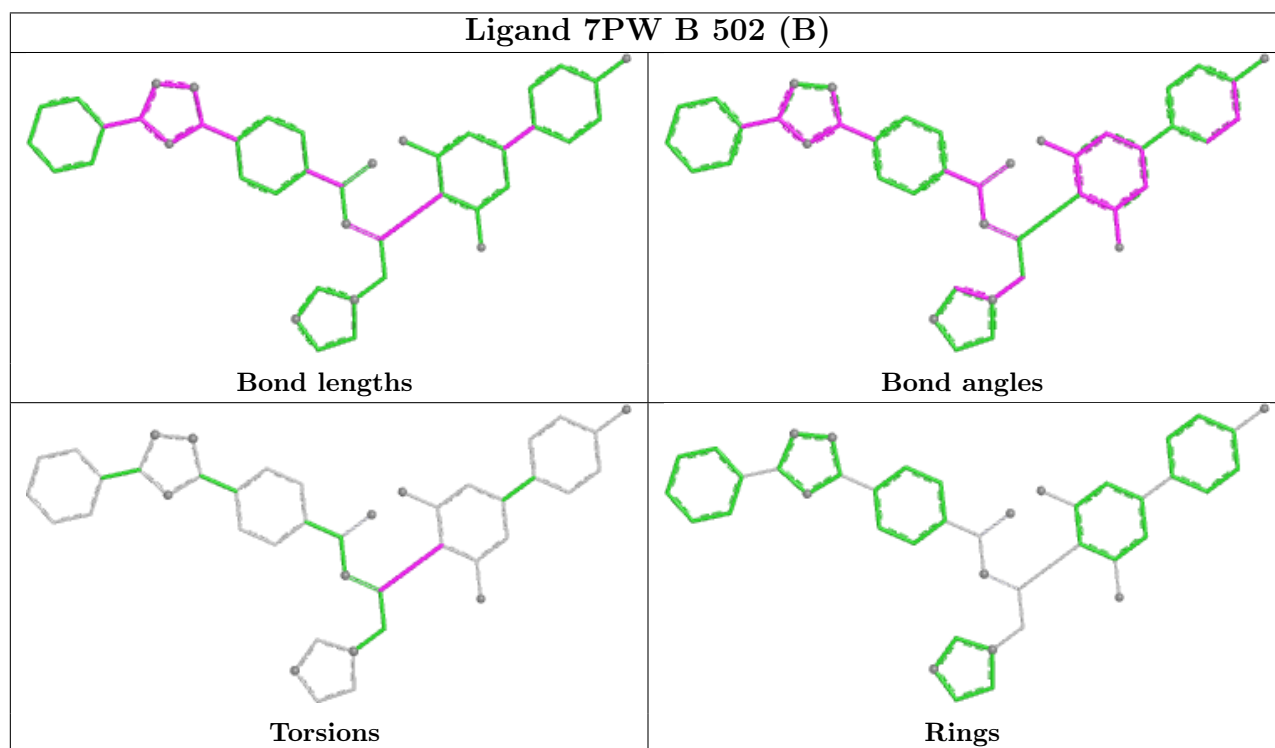
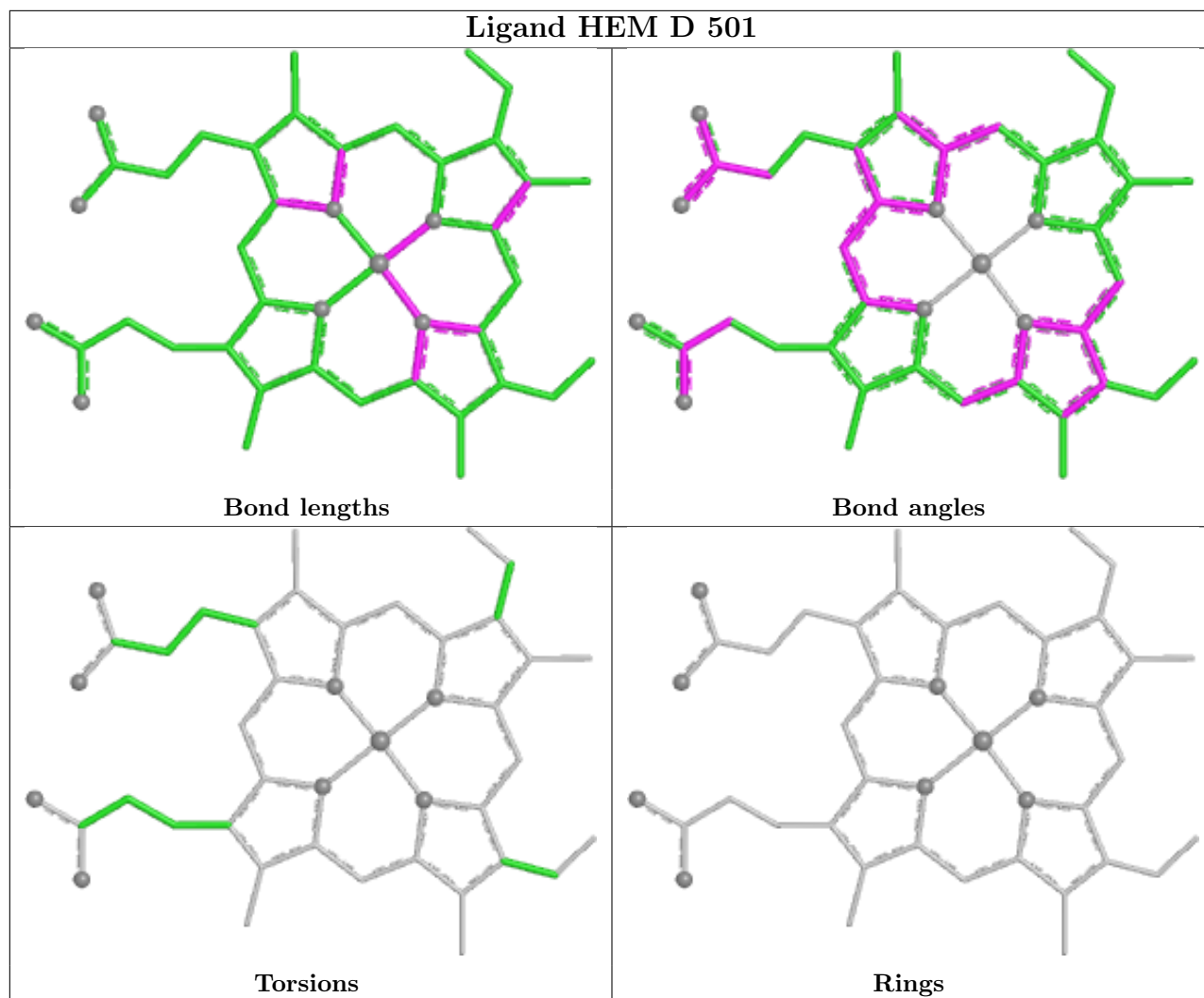


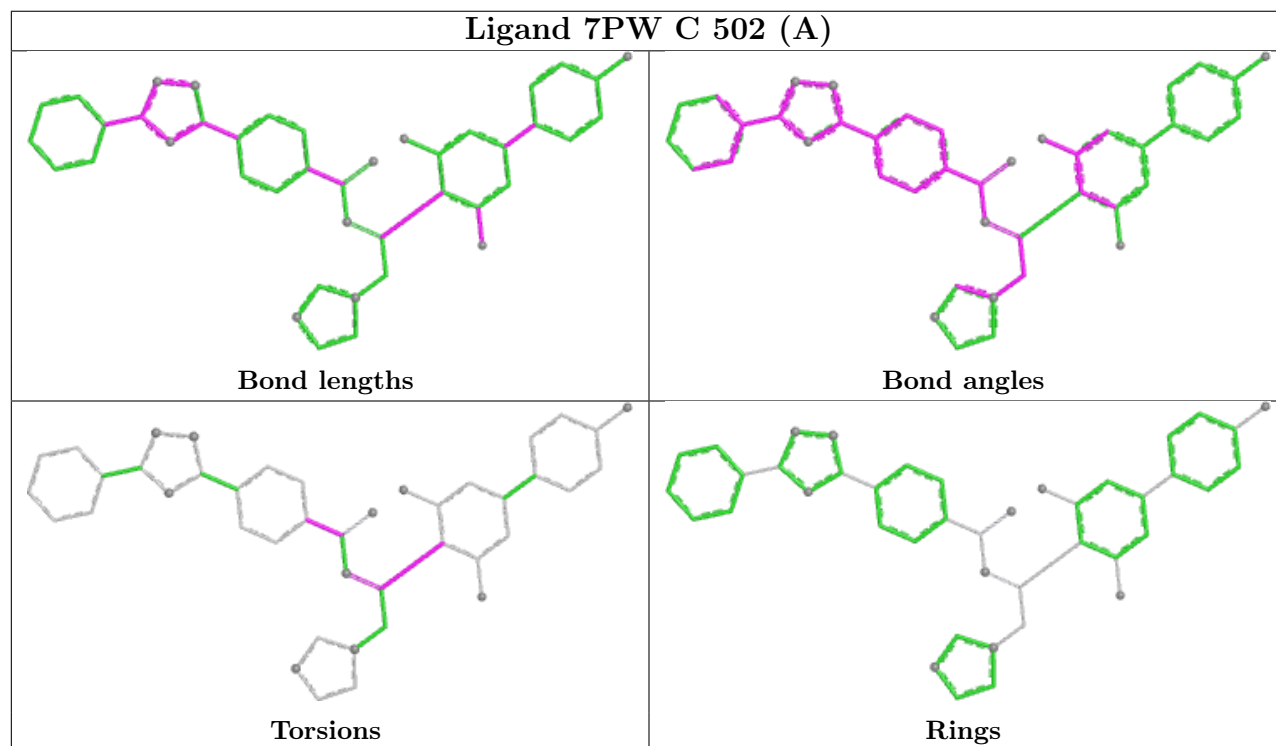
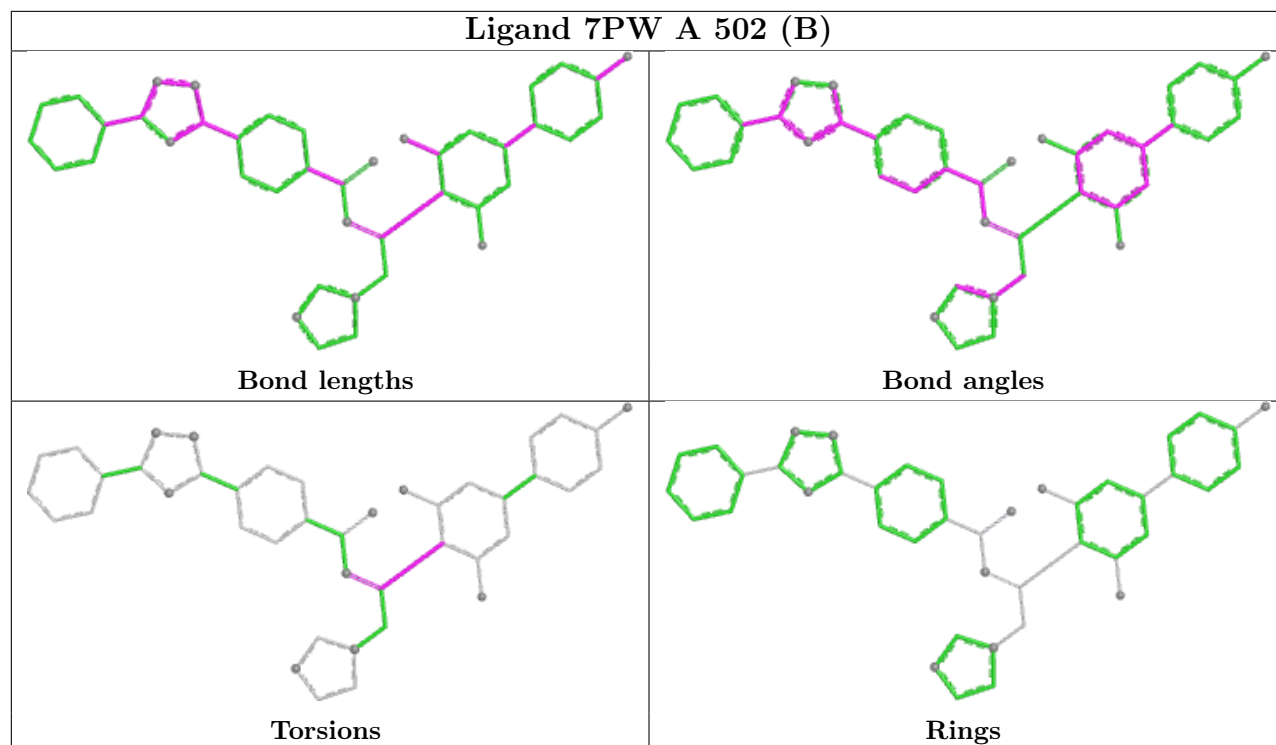


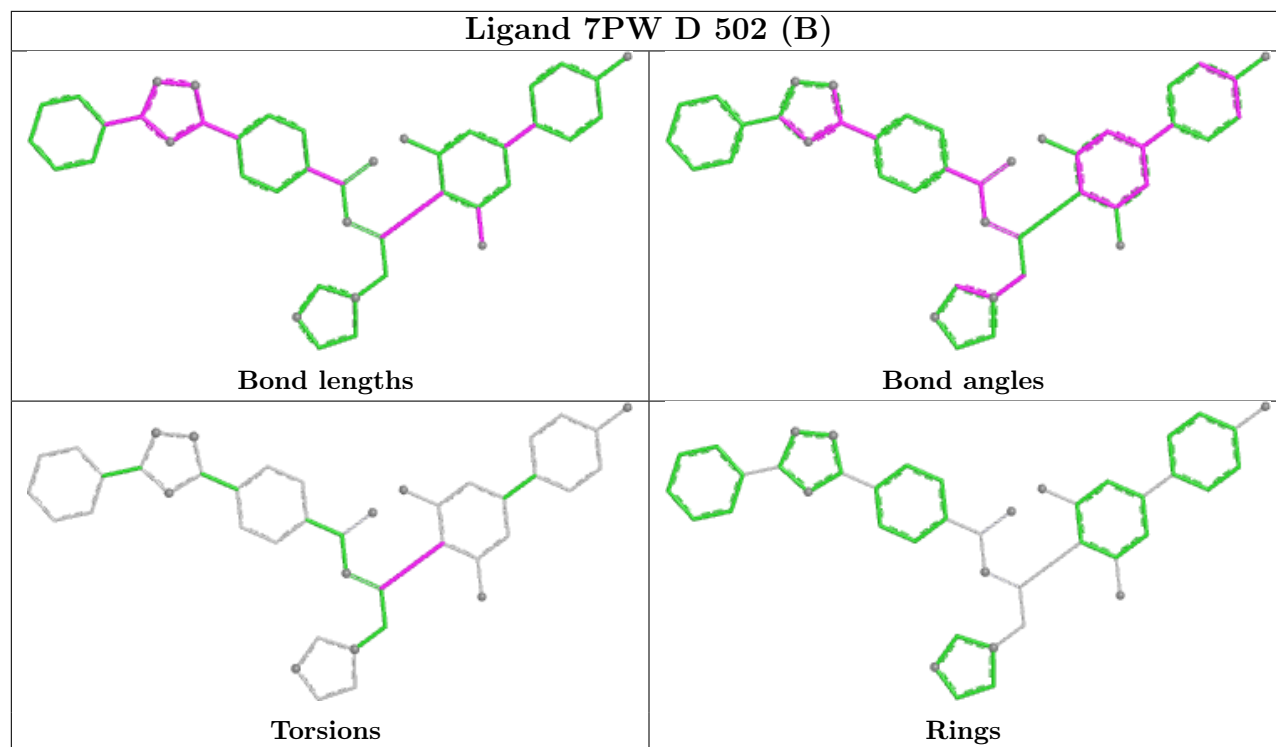












5.7 Other polymers [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	449/466 (96%)	0.27	18 (4%) 42 45	12, 27, 56, 100	0
1	B	449/466 (96%)	0.15	17 (3%) 44 47	11, 25, 52, 100	0
1	C	449/466 (96%)	0.28	22 (4%) 35 37	12, 27, 56, 99	0
1	D	449/466 (96%)	0.27	20 (4%) 38 41	12, 26, 56, 98	0
All	All	1796/1864 (96%)	0.25	77 (4%) 40 42	11, 26, 56, 100	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	222	PRO	5.6
1	C	222	PRO	4.6
1	A	222	PRO	4.3
1	A	473	PRO	4.2
1	D	473	PRO	4.2
1	A	43	LEU	4.1
1	A	44	ILE	4.0
1	B	219	PRO	4.0
1	B	222	PRO	3.9
1	C	213	PRO	3.9
1	C	219	PRO	3.9
1	B	221	LEU	3.8
1	A	221	LEU	3.7
1	D	43	LEU	3.6
1	D	220	SER	3.6
1	A	111	ARG	3.5
1	C	44	ILE	3.5
1	C	43	LEU	3.4
1	C	110	MET	3.3
1	A	219	PRO	3.3
1	B	214	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	220	SER	3.2
1	C	220	SER	3.2
1	B	44	ILE	3.1
1	D	221	LEU	3.1
1	C	473	PRO	3.1
1	A	110	MET	3.0
1	C	111	ARG	3.0
1	D	472	SER	3.0
1	D	51	VAL	3.0
1	C	210	GLY	3.0
1	A	204	TYR	3.0
1	C	221	LEU	2.9
1	B	229	ALA	2.9
1	A	95	LYS	2.8
1	D	474	PRO	2.8
1	C	215	SER	2.7
1	C	218	TYR	2.7
1	D	111	ARG	2.7
1	D	219	PRO	2.7
1	A	220	SER	2.7
1	A	211	ILE	2.6
1	A	205	HIS	2.6
1	A	218	TYR	2.5
1	B	95	LYS	2.5
1	B	472	SER	2.5
1	D	203	LEU	2.5
1	B	473	PRO	2.4
1	D	213	PRO	2.4
1	A	214	LEU	2.4
1	A	47	VAL	2.4
1	B	474	PRO	2.4
1	C	41	PRO	2.4
1	B	483	LYS	2.4
1	C	472	SER	2.4
1	C	51	VAL	2.4
1	D	211	ILE	2.4
1	C	95	LYS	2.4
1	D	204	TYR	2.3
1	C	205	HIS	2.3
1	D	110	MET	2.3
1	C	109	PHE	2.3
1	C	214	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	483	LYS	2.2
1	D	44	ILE	2.2
1	D	112	PRO	2.2
1	B	43	LEU	2.2
1	A	213	PRO	2.1
1	C	483	LYS	2.1
1	C	474	PRO	2.1
1	B	126	GLU	2.1
1	B	376	ILE	2.1
1	B	51	VAL	2.1
1	D	214	LEU	2.0
1	B	218	TYR	2.0
1	A	472	SER	2.0
1	D	68	TYR	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 oligosaccharides 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.

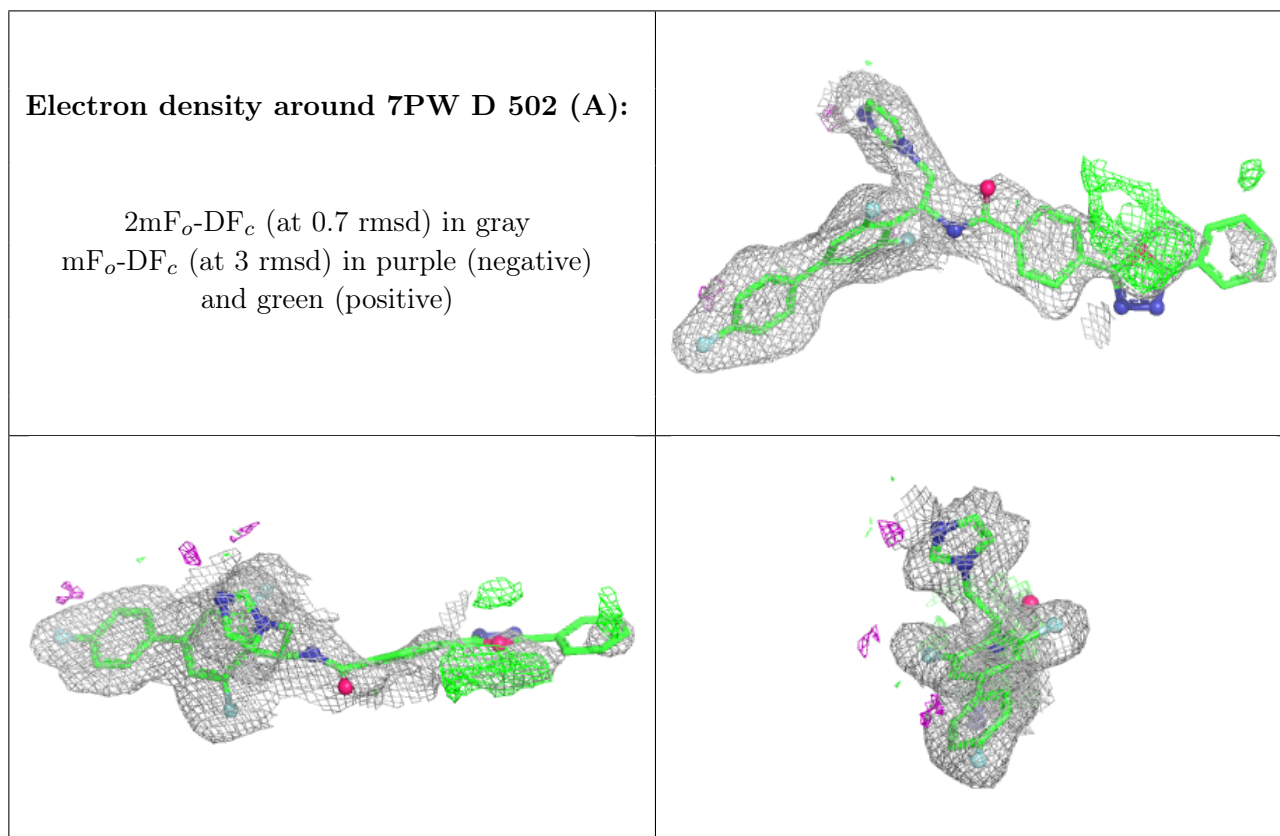
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	7PW	D	502[A]	42/42	0.83	0.20	17,24,54,56	42
3	7PW	D	502[B]	42/42	0.83	0.20	15,21,40,42	42
3	7PW	B	502[A]	42/42	0.85	0.16	15,19,43,47	42
3	7PW	B	502[B]	42/42	0.85	0.16	13,17,37,38	42
3	7PW	A	502[A]	42/42	0.85	0.16	17,22,45,46	42
3	7PW	A	502[B]	42/42	0.85	0.16	15,20,37,37	42
3	7PW	C	502[A]	42/42	0.88	0.14	16,22,44,47	42
3	7PW	C	502[B]	42/42	0.88	0.14	14,20,36,40	42
2	HEM	C	501	43/43	0.96	0.08	10,12,16,18	0

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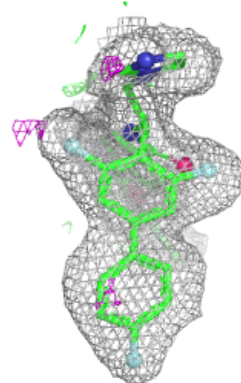
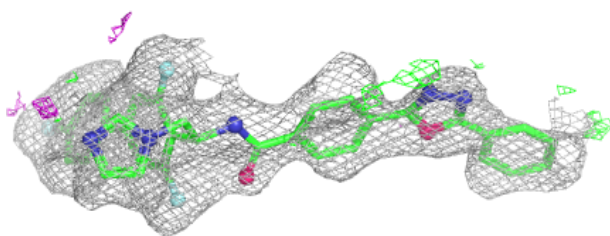
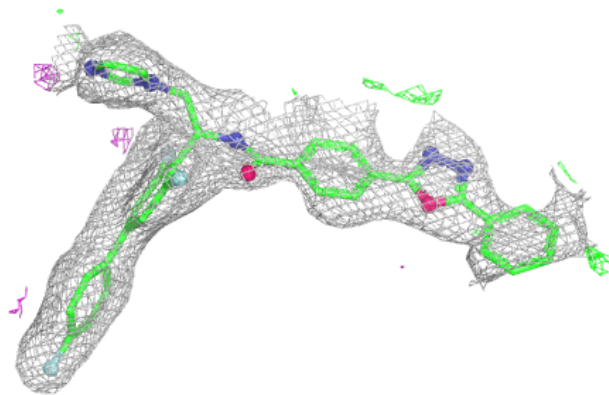
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	HEM	D	501	43/43	0.97	0.07	8,10,15,18	0
2	HEM	B	501	43/43	0.97	0.07	8,10,14,17	0
2	HEM	A	501	43/43	0.97	0.06	8,10,16,17	0

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.

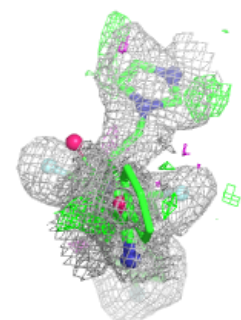
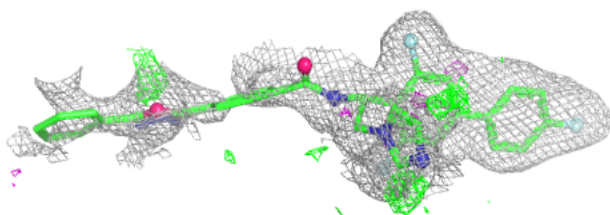
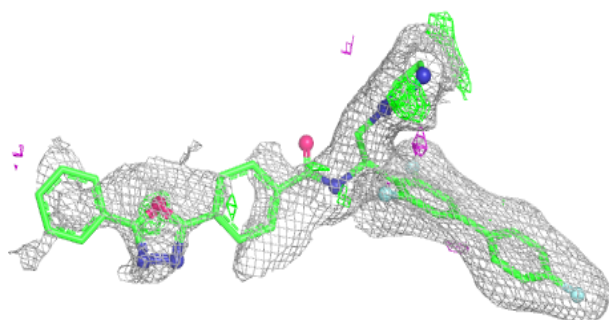


Electron density around 7PW D 502 (B):

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

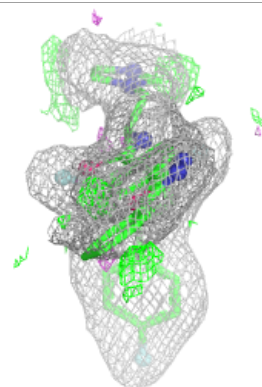
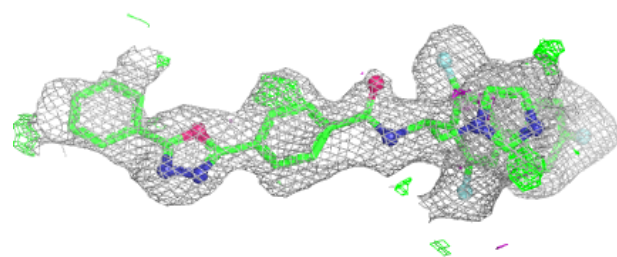
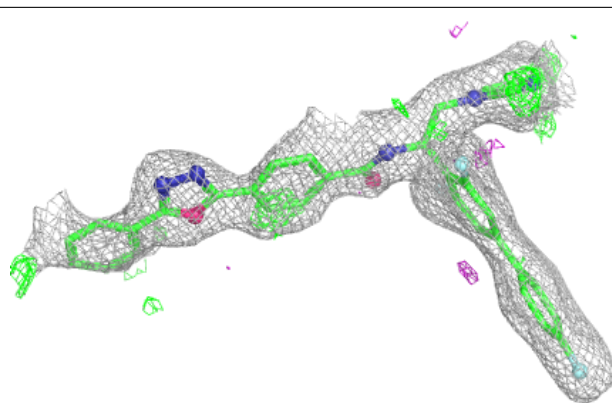
**Electron density around 7PW B 502 (A):**

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

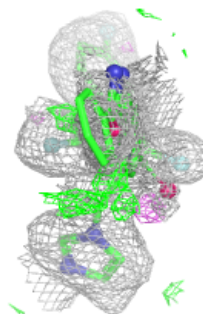
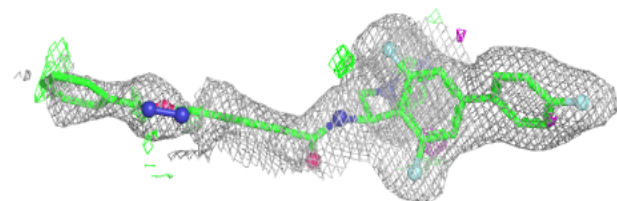
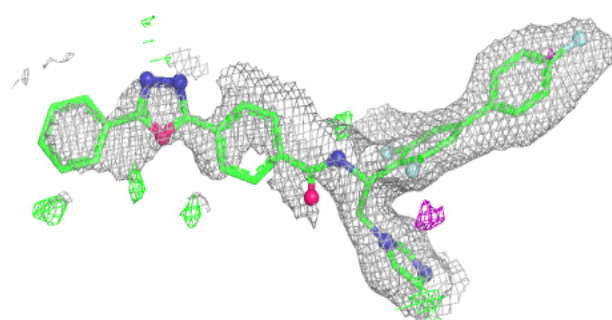


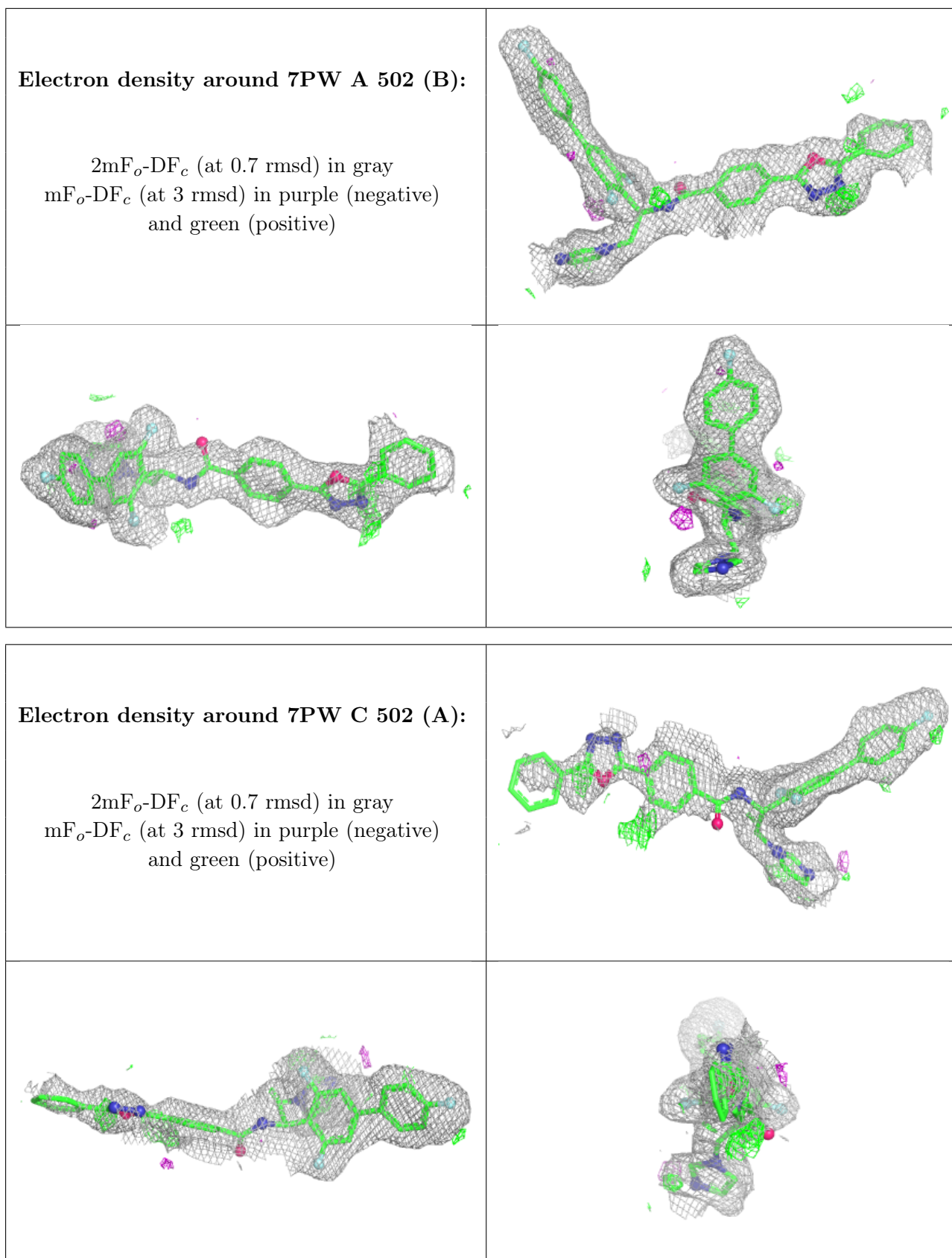
Electron density around 7PW B 502 (B):

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

**Electron density around 7PW A 502 (A):**

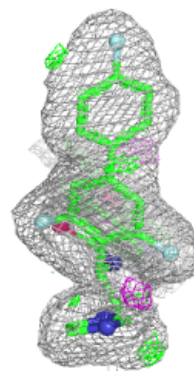
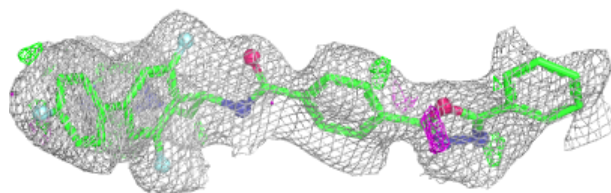
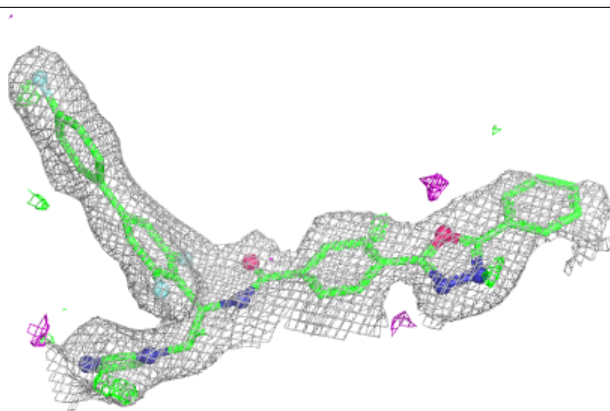
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



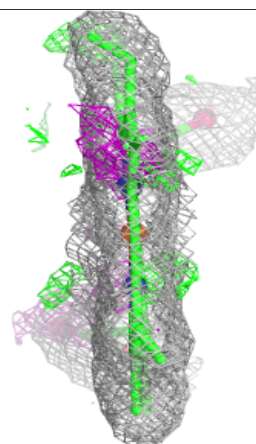
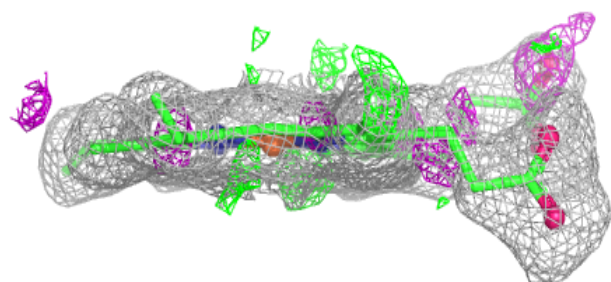
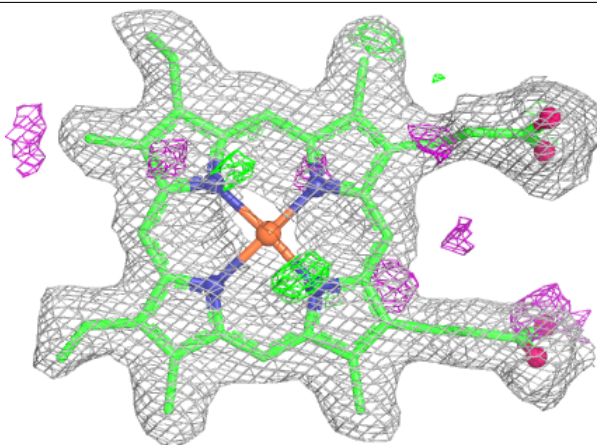


Electron density around 7PW C 502 (B):

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

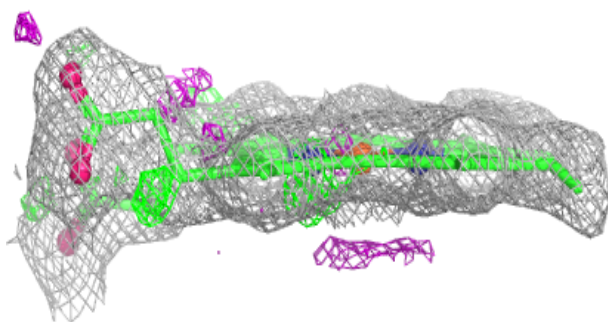
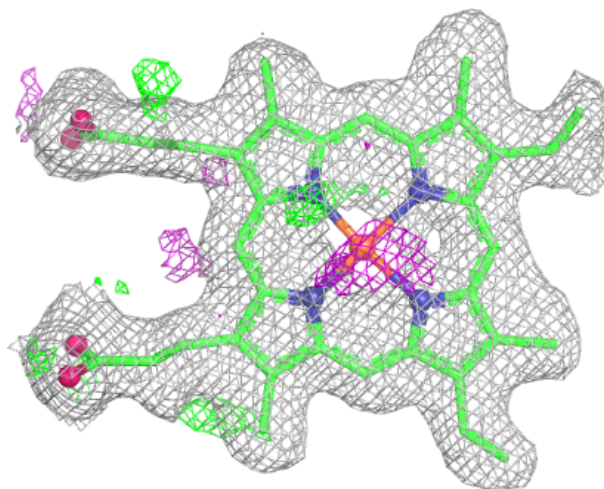
**Electron density around HEM C 501:**

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



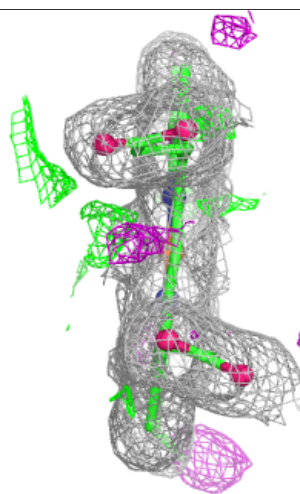
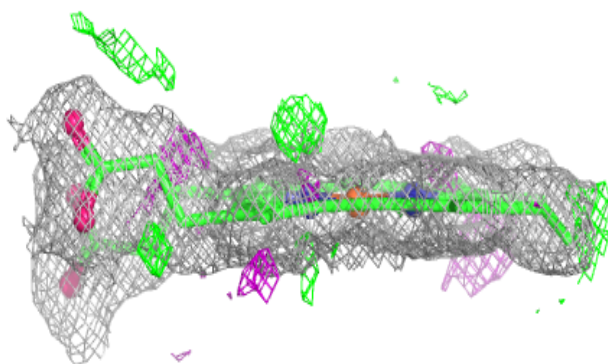
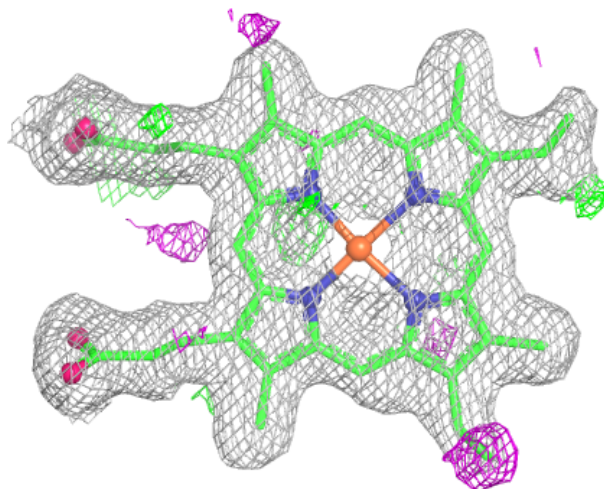
Electron density around HEM D 501:

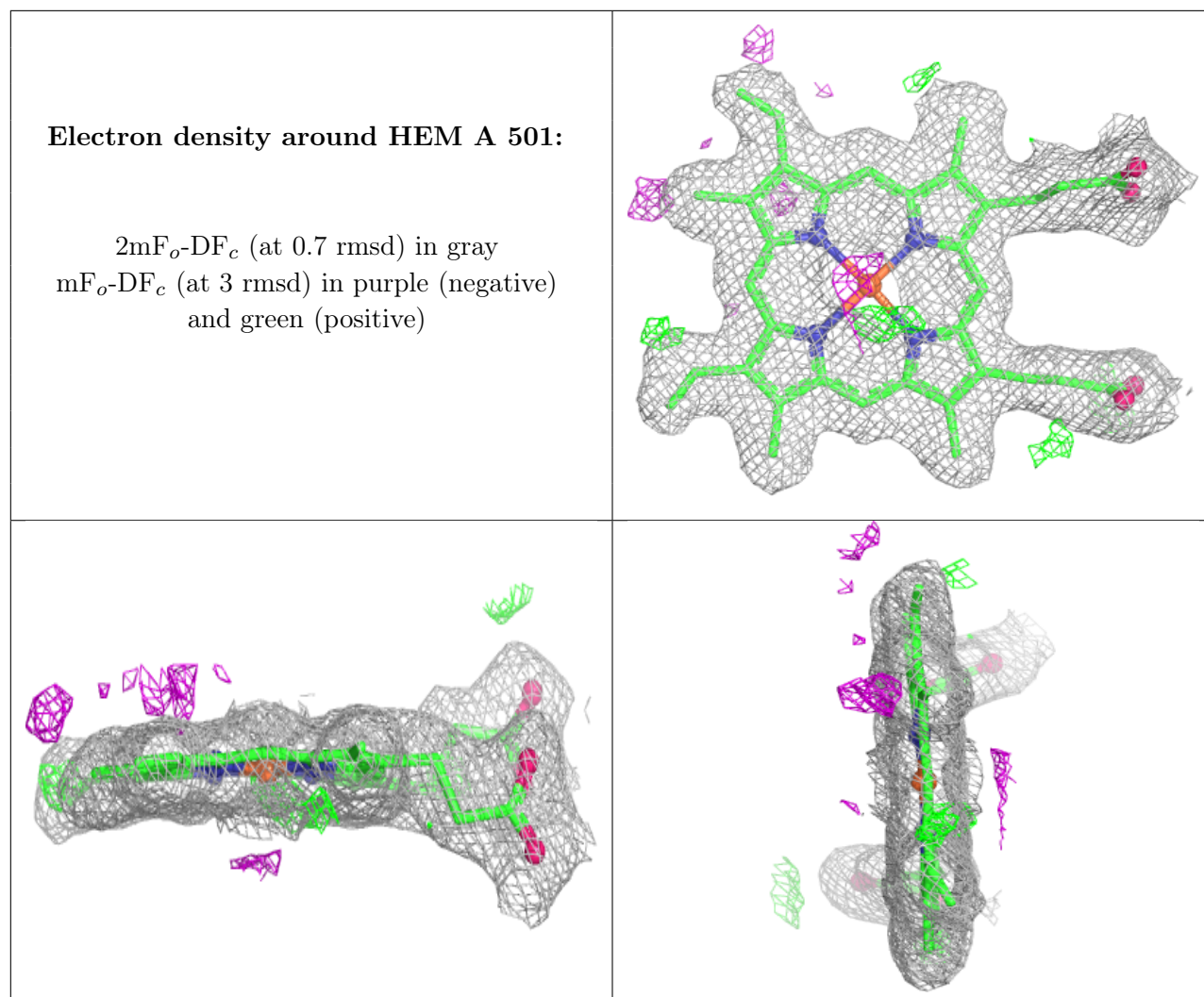
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.