



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 01:55 AM UTC

PDB ID : 9S7F / pdb_00009s7f
Title : Crystal structure of DoxA in complex with substrate DOD
Authors : Kim, R.Q.; Metsa-Ketela, M.
Deposited on : 2025-08-04
Resolution : 1.77 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)
Xtriage (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

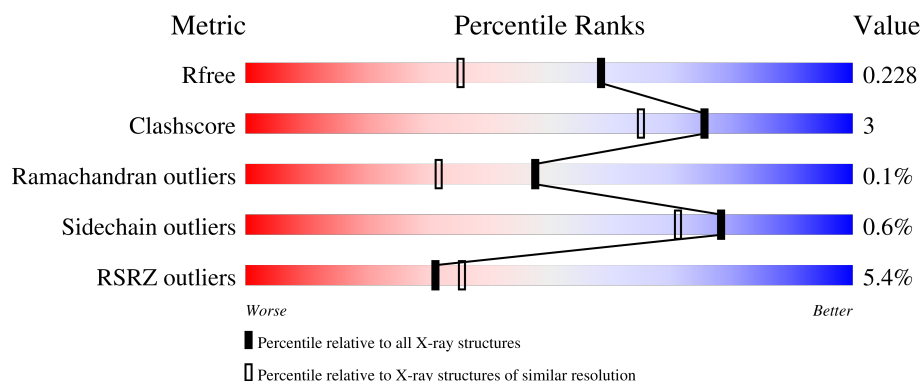
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	457	5% 76% 12% 11%
1	D	457	4% 80% 9% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6775 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 Cytochrome P-450 monooxygenase DoxA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	0	0
			3139	1986	572	570	11			
1	D	406	Total	C	N	O	S	0	0	0
			3134	1983	571	569	11			

There are 86 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-34	MET	-	initiating methionine	UNP Q9ZAU3
A	-33	GLY	-	expression tag	UNP Q9ZAU3
A	-32	GLY	-	expression tag	UNP Q9ZAU3
A	-31	SER	-	expression tag	UNP Q9ZAU3
A	-30	HIS	-	expression tag	UNP Q9ZAU3
A	-29	HIS	-	expression tag	UNP Q9ZAU3
A	-28	HIS	-	expression tag	UNP Q9ZAU3
A	-27	HIS	-	expression tag	UNP Q9ZAU3
A	-26	HIS	-	expression tag	UNP Q9ZAU3
A	-25	HIS	-	expression tag	UNP Q9ZAU3
A	-24	GLY	-	expression tag	UNP Q9ZAU3
A	-23	MET	-	expression tag	UNP Q9ZAU3
A	-22	ALA	-	expression tag	UNP Q9ZAU3
A	-21	SER	-	expression tag	UNP Q9ZAU3
A	-20	MET	-	expression tag	UNP Q9ZAU3
A	-19	THR	-	expression tag	UNP Q9ZAU3
A	-18	GLY	-	expression tag	UNP Q9ZAU3
A	-17	GLY	-	expression tag	UNP Q9ZAU3
A	-16	GLN	-	expression tag	UNP Q9ZAU3
A	-15	GLN	-	expression tag	UNP Q9ZAU3
A	-14	MET	-	expression tag	UNP Q9ZAU3
A	-13	GLY	-	expression tag	UNP Q9ZAU3
A	-12	ARG	-	expression tag	UNP Q9ZAU3
A	-11	ASP	-	expression tag	UNP Q9ZAU3
A	-10	LEU	-	expression tag	UNP Q9ZAU3

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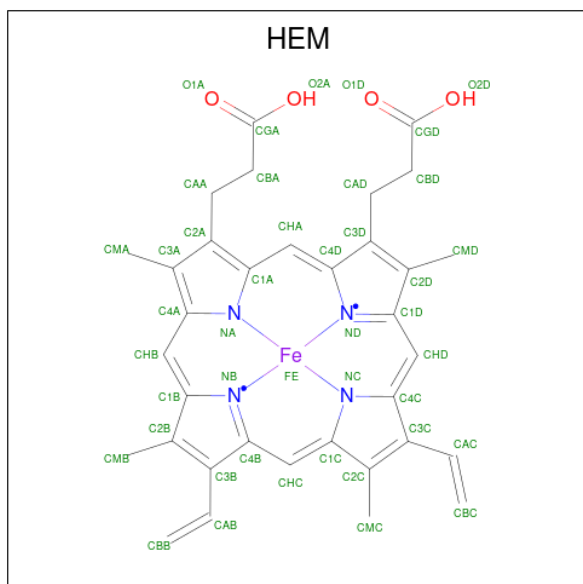
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	TYR	-	expression tag	UNP Q9ZAU3
A	-8	ASP	-	expression tag	UNP Q9ZAU3
A	-7	ASP	-	expression tag	UNP Q9ZAU3
A	-6	ASP	-	expression tag	UNP Q9ZAU3
A	-5	ASP	-	expression tag	UNP Q9ZAU3
A	-4	LYS	-	expression tag	UNP Q9ZAU3
A	-3	ASP	-	expression tag	UNP Q9ZAU3
A	-2	PRO	-	expression tag	UNP Q9ZAU3
A	-1	SER	-	expression tag	UNP Q9ZAU3
A	0	SER	-	expression tag	UNP Q9ZAU3
A	1	ARG	-	expression tag	UNP Q9ZAU3
A	2	SER	-	expression tag	UNP Q9ZAU3
A	3	GLY	-	expression tag	UNP Q9ZAU3
A	4	GLU	-	expression tag	UNP Q9ZAU3
A	5	ALA	-	expression tag	UNP Q9ZAU3
A	6	PRO	-	expression tag	UNP Q9ZAU3
A	7	ARG	-	expression tag	UNP Q9ZAU3
A	8	VAL	-	expression tag	UNP Q9ZAU3
D	-34	MET	-	initiating methionine	UNP Q9ZAU3
D	-33	GLY	-	expression tag	UNP Q9ZAU3
D	-32	GLY	-	expression tag	UNP Q9ZAU3
D	-31	SER	-	expression tag	UNP Q9ZAU3
D	-30	HIS	-	expression tag	UNP Q9ZAU3
D	-29	HIS	-	expression tag	UNP Q9ZAU3
D	-28	HIS	-	expression tag	UNP Q9ZAU3
D	-27	HIS	-	expression tag	UNP Q9ZAU3
D	-26	HIS	-	expression tag	UNP Q9ZAU3
D	-25	HIS	-	expression tag	UNP Q9ZAU3
D	-24	GLY	-	expression tag	UNP Q9ZAU3
D	-23	MET	-	expression tag	UNP Q9ZAU3
D	-22	ALA	-	expression tag	UNP Q9ZAU3
D	-21	SER	-	expression tag	UNP Q9ZAU3
D	-20	MET	-	expression tag	UNP Q9ZAU3
D	-19	THR	-	expression tag	UNP Q9ZAU3
D	-18	GLY	-	expression tag	UNP Q9ZAU3
D	-17	GLY	-	expression tag	UNP Q9ZAU3
D	-16	GLN	-	expression tag	UNP Q9ZAU3
D	-15	GLN	-	expression tag	UNP Q9ZAU3
D	-14	MET	-	expression tag	UNP Q9ZAU3
D	-13	GLY	-	expression tag	UNP Q9ZAU3
D	-12	ARG	-	expression tag	UNP Q9ZAU3
D	-11	ASP	-	expression tag	UNP Q9ZAU3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	LEU	-	expression tag	UNP Q9ZAU3
D	-9	TYR	-	expression tag	UNP Q9ZAU3
D	-8	ASP	-	expression tag	UNP Q9ZAU3
D	-7	ASP	-	expression tag	UNP Q9ZAU3
D	-6	ASP	-	expression tag	UNP Q9ZAU3
D	-5	ASP	-	expression tag	UNP Q9ZAU3
D	-4	LYS	-	expression tag	UNP Q9ZAU3
D	-3	ASP	-	expression tag	UNP Q9ZAU3
D	-2	PRO	-	expression tag	UNP Q9ZAU3
D	-1	SER	-	expression tag	UNP Q9ZAU3
D	0	SER	-	expression tag	UNP Q9ZAU3
D	1	ARG	-	expression tag	UNP Q9ZAU3
D	2	SER	-	expression tag	UNP Q9ZAU3
D	3	GLY	-	expression tag	UNP Q9ZAU3
D	4	GLU	-	expression tag	UNP Q9ZAU3
D	5	ALA	-	expression tag	UNP Q9ZAU3
D	6	PRO	-	expression tag	UNP Q9ZAU3
D	7	ARG	-	expression tag	UNP Q9ZAU3
D	8	VAL	-	expression tag	UNP Q9ZAU3

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



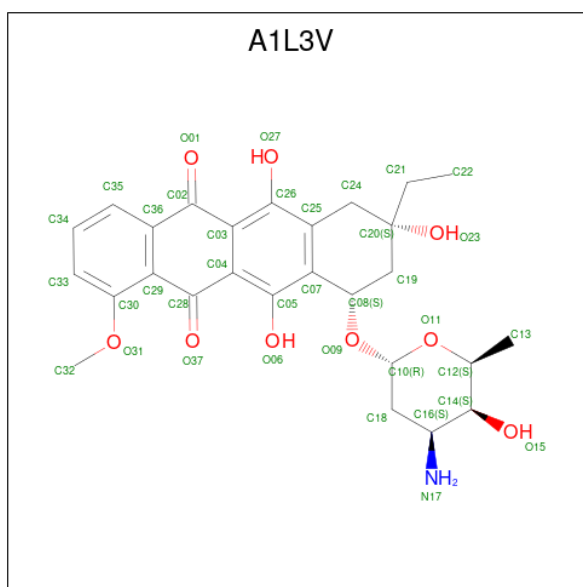
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
							0	0

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

- Molecule 3 is (7 {S},9 {S})-7-[(2 {R},4 {S},5 {S},6 {S})-4-azanyl-6-methyl-5-oxidanyl-oxan-2-yl]oxy-9-ethyl-4-methoxy-6,9,11-tris(oxidanyl)-8,10-dihydro-7 {H}-tetracene-5,12-dione (CCD ID: A1L3V) (formula: C₂₇H₃₁NO₉) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			37	27	1	9		
3	D	1	Total	C	N	O	0	0
			37	27	1	9		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	183	Total	O	0	0
			183	183		
4	D	159	Total	O	0	0
			159	159		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	101.75Å 107.71Å 184.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.08 – 1.77 74.08 – 1.77	Depositor EDS
% Data completeness (in resolution range)	98.8 (74.08-1.77) 97.9 (74.08-1.77)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.105)	Depositor
R, R_{free}	0.194 , 0.222 0.200 , 0.228	Depositor DCC
R_{free} test set	4820 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6775	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, A1L3V

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	3/3218 (0.1%)	1.47	26/4386 (0.6%)
1	D	0.94	2/3213 (0.1%)	1.38	14/4379 (0.3%)
All	All	0.98	5/6431 (0.1%)	1.43	40/8765 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	D	0	9
All	All	0	13

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	346	ALA	C-O	-8.78	1.19	1.23
1	D	380	ARG	NE-CZ	6.84	1.40	1.33
1	A	225	ARG	NE-CZ	6.28	1.40	1.33
1	A	380	ARG	NE-CZ	6.18	1.39	1.33
1	A	144	SER	CA-CB	-5.81	1.44	1.53

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	GLN	CG-CD-NE2	-8.18	104.13	116.40
1	D	340	ASP	CA-CB-CG	7.57	120.17	112.60
1	D	79	VAL	N-CA-CB	-7.16	105.77	111.64
1	A	348	HIS	CB-CG-CD2	7.12	140.46	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	ALA	CA-C-N	7.04	126.74	119.56
1	A	346	ALA	C-N-CA	7.04	126.74	119.56
1	A	260	PHE	CA-CB-CG	-6.69	107.11	113.80
1	A	418	PRO	CB-CA-C	6.67	117.47	111.40
1	A	143	ARG	CB-CA-C	-6.66	98.50	110.70
1	A	287	ASP	CA-CB-CG	6.62	119.22	112.60
1	D	25	GLU	CB-CG-CD	6.55	123.74	112.60
1	A	139	ASP	CA-CB-CG	6.45	119.05	112.60
1	D	311	ARG	CD-NE-CZ	6.11	132.95	124.40
1	A	348	HIS	CB-CG-ND1	-6.10	113.55	122.70
1	A	224	ARG	CB-CA-C	-6.09	97.96	110.38
1	A	397	VAL	O-C-N	-6.07	117.47	121.72
1	A	249	ASP	CA-CB-CG	6.04	118.64	112.60
1	D	410	GLN	CB-CA-C	-5.98	98.53	109.54
1	D	354	ARG	N-CA-CB	-5.83	100.83	109.98
1	D	380	ARG	CG-CD-NE	5.76	124.67	112.00
1	D	265	THR	OG1-CB-CG2	-5.75	97.80	109.30
1	A	376	GLN	CA-C-O	-5.65	114.88	120.82
1	A	387	ARG	CG-CD-NE	-5.64	99.59	112.00
1	A	158	PHE	O-C-N	-5.56	115.99	120.38
1	A	311	ARG	NE-CZ-NH1	5.54	127.04	121.50
1	D	176	MET	CG-SD-CE	5.48	112.96	100.90
1	A	378	GLU	CA-C-N	5.42	127.80	120.65
1	A	378	GLU	C-N-CA	5.42	127.80	120.65
1	A	32	GLU	CB-CG-CD	5.38	121.75	112.60
1	D	62	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	422	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	A	288	GLU	CB-CG-CD	5.23	121.49	112.60
1	A	373	GLN	N-CA-CB	5.20	117.86	110.16
1	A	64	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	D	361	THR	OG1-CB-CG2	5.15	119.61	109.30
1	A	28	ASP	N-CA-C	-5.12	105.39	111.69
1	D	315	THR	CA-CB-OG1	-5.12	101.92	109.60
1	D	387	ARG	CD-NE-CZ	5.11	131.56	124.40
1	A	376	GLN	CB-CG-CD	5.08	121.25	112.60
1	D	269	PHE	CA-CB-CG	-5.01	108.79	113.80

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	225	ARG	Sidechain
1	A	387	ARG	Sidechain
1	A	389	ARG	Sidechain
1	D	122	ARG	Sidechain
1	D	125	ARG	Sidechain
1	D	132	ARG	Sidechain
1	D	22	ARG	Sidechain
1	D	224	ARG	Sidechain
1	D	233	ARG	Sidechain
1	D	281	ARG	Sidechain
1	D	394	ARG	Sidechain
1	D	77	ARG	Sidechain

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	3139	0	3112	25	0
1	D	3134	0	3107	12	0
2	A	43	0	30	1	0
2	D	43	0	30	0	0
3	A	37	0	0	1	0
3	D	37	0	0	1	0
4	A	183	0	0	5	0
4	D	159	0	0	4	0
All	All	6775	0	6279	38	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 (38) 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:A:351:HIS:HD2	4:A:769:HOH:O	1.71	0.71
1:A:50:ILE:HD13	1:A:59:VAL:HG21	1.77	0.67
1:A:111:ALA:HB3	1:A:112:PRO:HD3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:LYS:O	1:A:410:GLN:HG2	1.96	0.66
1:A:357:TRP:NE1	4:A:601:HOH:O	2.15	0.65
1:A:115:ASN:HB3	1:A:118:ARG:HD3	1.81	0.61
1:A:407:LYS:HG2	1:A:410:GLN:NE2	2.19	0.57
1:D:157:HIS:HE1	4:D:742:HOH:O	1.87	0.57
1:A:50:ILE:CD1	1:A:59:VAL:HG21	2.37	0.54
1:A:125:ARG:HG2	1:A:165:GLU:OE2	2.08	0.53
1:A:221:HIS:HE1	4:A:611:HOH:O	1.91	0.53
3:D:502:A1L3V:O01	3:D:502:A1L3V:O27	2.29	0.50
1:D:111:ALA:HB3	1:D:112:PRO:HD3	1.94	0.49
1:A:383:ILE:O	1:A:387:ARG:HG2	2.13	0.49
1:A:407:LYS:H	1:A:410:GLN:NE2	2.10	0.49
1:A:143:ARG:HB3	1:D:292:SER:HB2	1.95	0.47
1:A:77:ARG:N	1:A:77:ARG:HD2	2.28	0.47
1:D:351:HIS:HD2	4:D:625:HOH:O	1.98	0.47
1:A:170:PRO:HG2	1:A:215:LEU:HD22	1.96	0.47
1:D:80:ASP:O	1:D:82:GLY:N	2.44	0.45
1:A:420:TRP:CZ2	1:D:116:PRO:HB2	2.51	0.45
1:D:20:MET:SD	1:D:414:LEU:HD21	2.56	0.45
1:D:268:SER:HB3	1:D:412:ALA:O	2.16	0.45
1:D:319:ILE:HD11	1:D:324:LEU:HD11	2.00	0.44
1:A:67:LYS:O	1:A:68:ASP:C	2.62	0.43
1:A:357:TRP:O	1:A:359:ARG:NH1	2.51	0.43
1:D:380:ARG:CG	4:D:624:HOH:O	2.66	0.43
1:A:103:HIS:CD2	1:A:367:HIS:CE1	3.06	0.43
1:D:357:TRP:O	1:D:359:ARG:NH2	2.52	0.42
1:A:77:ARG:HD2	1:A:77:ARG:H	1.84	0.42
1:A:118:ARG:HD2	4:A:655:HOH:O	2.20	0.42
1:A:91:ARG:N	1:A:92:PRO:CD	2.83	0.42
1:A:8:VAL:HG12	1:A:10:VAL:HG22	2.02	0.42
1:A:218:GLU:OE1	4:A:602:HOH:O	2.22	0.42
3:A:502:A1L3V:O01	3:A:502:A1L3V:O27	2.37	0.41
1:A:112:PRO:HB2	1:A:234:VAL:HG11	2.03	0.41
1:D:380:ARG:HG3	4:D:624:HOH:O	2.20	0.41
2:A:501:HEM:HBB2	2:A:501:HEM:CMB	2.51	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	402/457 (88%)	395 (98%)	6 (2%)	1 (0%)	43	27
1	D	402/457 (88%)	397 (99%)	5 (1%)	0	100	100
All	All	804/914 (88%)	792 (98%)	11 (1%)	1 (0%)	48	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	PRO

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	322/358 (90%)	319 (99%)	3 (1%)	70	60
1	D	321/358 (90%)	320 (100%)	1 (0%)	86	83
All	All	643/716 (90%)	639 (99%)	4 (1%)	78	71

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	79	VAL
1	A	319	ILE
1	D	81	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	240	GLN
1	A	376	GLN
1	A	410	GLN
1	D	221	HIS
1	D	240	GLN
1	D	343	HIS
1	D	344	HIS

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](#)

4 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	A1L3V	A	502	-	41,41,41	1.40	5 (12%)	57,64,64	1.41	7 (12%)
2	HEM	A	501	1	50,50,50	2.77	18 (36%)	67,82,82	3.26	29 (43%)
2	HEM	D	501	1	50,50,50	2.19	16 (32%)	67,82,82	2.09	19 (28%)
3	A1L3V	D	502	-	41,41,41	1.10	3 (7%)	57,64,64	1.16	5 (8%)

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	A1L3V	A	502	-	-	0/9/55/55	0/5/5/5
2	HEM	A	501	1	-	2/14/54/54	-
2	HEM	D	501	1	-	2/14/54/54	-
3	A1L3V	D	502	-	-	1/9/55/55	0/5/5/5

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	FE-NA	8.20	2.22	1.95
2	A	501	HEM	FE-NC	8.15	2.22	1.95
2	D	501	HEM	FE-NB	6.31	2.14	1.94
2	A	501	HEM	CHB-C1B	5.88	1.50	1.38
2	D	501	HEM	FE-ND	5.54	2.12	1.94
2	D	501	HEM	FE-NC	5.36	2.12	1.95
2	A	501	HEM	C4D-ND	5.22	1.49	1.40
2	A	501	HEM	C4A-NA	-4.98	1.30	1.39
2	D	501	HEM	C1B-NB	-4.89	1.31	1.40
2	A	501	HEM	C4D-C3D	-4.18	1.37	1.45
3	A	502	A1L3V	O23-C20	3.93	1.52	1.44
2	A	501	HEM	C4C-NC	-3.84	1.32	1.39
2	A	501	HEM	C3B-C4B	-3.80	1.37	1.44
2	A	501	HEM	CHC-C1C	-3.64	1.31	1.38
3	A	502	A1L3V	C36-C02	-3.59	1.41	1.48
2	A	501	HEM	CBD-CGD	3.46	1.58	1.50
2	A	501	HEM	C1A-NA	-3.42	1.33	1.39
2	D	501	HEM	FE-NA	3.35	2.06	1.95
2	A	501	HEM	C4B-NB	3.28	1.45	1.38
2	A	501	HEM	CHD-C1D	3.25	1.46	1.39
3	A	502	A1L3V	C04-C28	-3.23	1.40	1.47
2	D	501	HEM	CHA-C4D	3.23	1.45	1.38
3	A	502	A1L3V	O09-C08	3.04	1.49	1.44
2	D	501	HEM	C4D-C3D	-3.02	1.39	1.45
3	D	502	A1L3V	O01-C02	2.92	1.28	1.22
2	D	501	HEM	C1A-NA	2.80	1.44	1.39
2	A	501	HEM	C1B-C2B	-2.78	1.38	1.44
2	D	501	HEM	C3B-C4B	-2.76	1.39	1.44
2	A	501	HEM	C4A-C3A	2.63	1.49	1.43
3	D	502	A1L3V	C03-C26	-2.62	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	CHD-C4C	2.57	1.43	1.38
2	D	501	HEM	C3C-C4C	-2.50	1.41	1.46
2	D	501	HEM	C4C-NC	-2.43	1.35	1.39
2	D	501	HEM	C1A-C2A	-2.33	1.39	1.44
3	D	502	A1L3V	C36-C29	2.33	1.44	1.41
2	A	501	HEM	CMC-C2C	2.24	1.55	1.50
3	A	502	A1L3V	O37-C28	2.19	1.26	1.22
2	D	501	HEM	C1C-NC	-2.14	1.35	1.39
2	A	501	HEM	CBA-CGA	2.13	1.55	1.50
2	D	501	HEM	CHD-C1D	2.08	1.43	1.39
2	A	501	HEM	O2A-CGA	-2.08	1.23	1.30
2	D	501	HEM	C4D-ND	-2.05	1.36	1.40

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C3B-C4B-NB	8.12	115.30	109.47
2	D	501	HEM	CHC-C4B-NB	-8.07	115.74	124.42
2	A	501	HEM	C4D-ND-C1D	-7.65	96.14	105.21
2	A	501	HEM	CHA-C4D-ND	-7.55	115.03	124.37
2	A	501	HEM	C2A-C1A-NA	-6.99	102.39	110.15
2	A	501	HEM	C4C-NC-C1C	6.50	116.41	105.82
2	A	501	HEM	C4A-NA-C1A	6.37	116.21	105.82
2	A	501	HEM	C1B-NB-C4B	-6.11	97.98	105.21
2	D	501	HEM	C1C-CHC-C4B	5.81	138.36	126.02
2	A	501	HEM	CHD-C1D-ND	-5.53	118.47	124.42
2	A	501	HEM	C2D-C1D-ND	5.52	116.28	109.90
2	A	501	HEM	CHC-C4B-NB	-5.30	118.72	124.42
3	A	502	A1L3V	O23-C20-C21	4.87	116.97	108.74
2	D	501	HEM	CHA-C4D-ND	-4.71	118.54	124.37
2	A	501	HEM	CMA-C3A-C2A	4.45	135.07	125.62
2	A	501	HEM	CHC-C1C-NC	4.45	129.29	124.45
2	A	501	HEM	C3D-C4D-ND	4.38	114.98	110.17
2	A	501	HEM	C2B-C1B-NB	4.21	114.68	109.84
2	D	501	HEM	CHC-C4B-C3B	4.17	133.40	125.07
2	D	501	HEM	CHD-C4C-NC	-4.10	119.99	124.45
2	A	501	HEM	O1D-CGD-CBD	-3.98	110.47	123.09
2	A	501	HEM	C1A-CHA-C4D	3.93	135.50	126.25
2	A	501	HEM	CHD-C4C-C3C	3.90	131.78	125.21
3	D	502	A1L3V	O23-C20-C21	3.90	115.32	108.74
2	D	501	HEM	C3C-C2C-C1C	-3.78	103.47	107.05
2	A	501	HEM	O2D-CGD-CBD	3.59	125.34	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	A1L3V	C19-C08-C07	3.56	119.08	110.71
2	D	501	HEM	C1D-C2D-C3D	-3.55	103.25	106.98
3	A	502	A1L3V	O06-C05-C04	-3.50	113.27	120.95
2	A	501	HEM	C1C-CHC-C4B	3.50	133.46	126.02
2	A	501	HEM	C4B-C3B-C2B	-3.43	104.13	107.28
2	D	501	HEM	C1A-CHA-C4D	3.42	134.29	126.25
2	A	501	HEM	C4A-C3A-C2A	-3.24	103.11	106.82
2	A	501	HEM	C4C-C3C-C2C	3.05	109.46	106.81
2	D	501	HEM	CHD-C1D-ND	-3.02	121.18	124.42
2	A	501	HEM	CHA-C1A-NA	2.99	129.29	123.86
3	D	502	A1L3V	O23-C20-C24	-2.95	101.94	108.42
2	D	501	HEM	CHD-C4C-C3C	2.91	130.12	125.21
2	D	501	HEM	CHA-C4D-C3D	2.80	130.40	125.23
2	A	501	HEM	C2C-C1C-NC	-2.78	104.49	109.64
3	D	502	A1L3V	O27-C26-C03	-2.76	114.91	120.95
2	D	501	HEM	CAC-C3C-C4C	-2.62	118.56	124.82
3	A	502	A1L3V	O27-C26-C03	-2.61	115.24	120.95
2	A	501	HEM	C1A-C2A-C3A	2.60	110.89	106.87
2	A	501	HEM	CHA-C4D-C3D	2.56	129.94	125.23
2	D	501	HEM	C2D-C1D-ND	2.53	112.83	109.90
3	A	502	A1L3V	O11-C12-C14	-2.41	105.22	109.55
2	A	501	HEM	CMA-C3A-C4A	-2.40	121.76	125.42
3	A	502	A1L3V	O23-C20-C19	-2.34	103.29	109.33
2	D	501	HEM	CHB-C4A-NA	-2.32	119.65	123.86
2	A	501	HEM	O1A-CGA-CBA	-2.23	116.02	123.09
2	D	501	HEM	C4D-C3D-C2D	2.17	110.05	106.89
2	A	501	HEM	CAD-C3D-C4D	2.17	128.48	124.70
2	D	501	HEM	C4B-C3B-C2B	-2.16	105.30	107.28
3	A	502	A1L3V	O06-C05-C07	2.15	124.54	119.02
2	D	501	HEM	CHA-C1A-C2A	2.12	129.94	125.30
3	D	502	A1L3V	O31-C30-C33	-2.10	120.76	124.30
2	D	501	HEM	C4C-CHD-C1D	2.02	130.32	126.02
3	D	502	A1L3V	O01-C02-C36	2.01	123.89	120.99
2	D	501	HEM	C4D-ND-C1D	-2.00	102.84	105.21

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	502	A1L3V	C19-C20-C21-C22
2	D	501	HEM	CAA-CBA-CGA-O1A
2	D	501	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
2	A	501	HEM	CAD-CBD-CGD-O1D
2	A	501	HEM	CAD-CBD-CGD-O2D

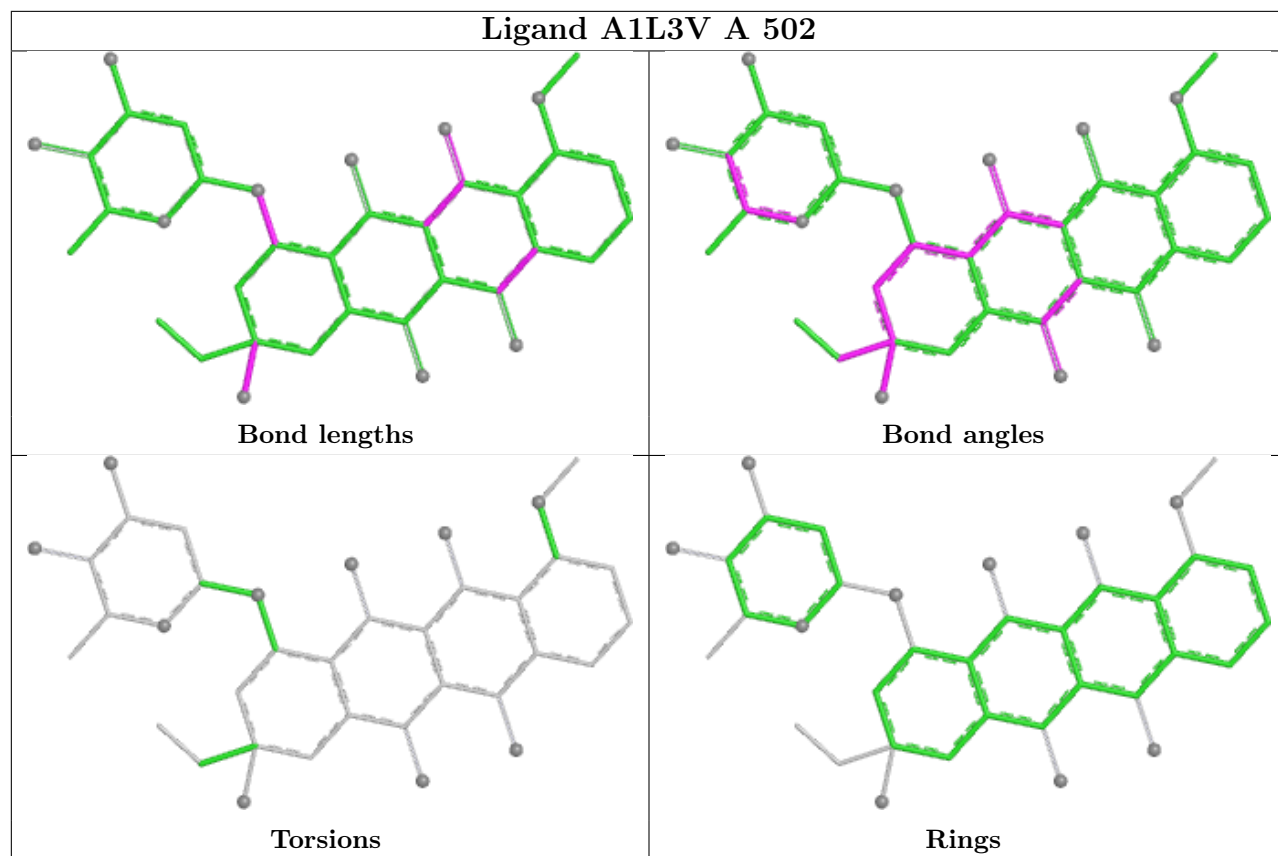
There are no ring outliers.

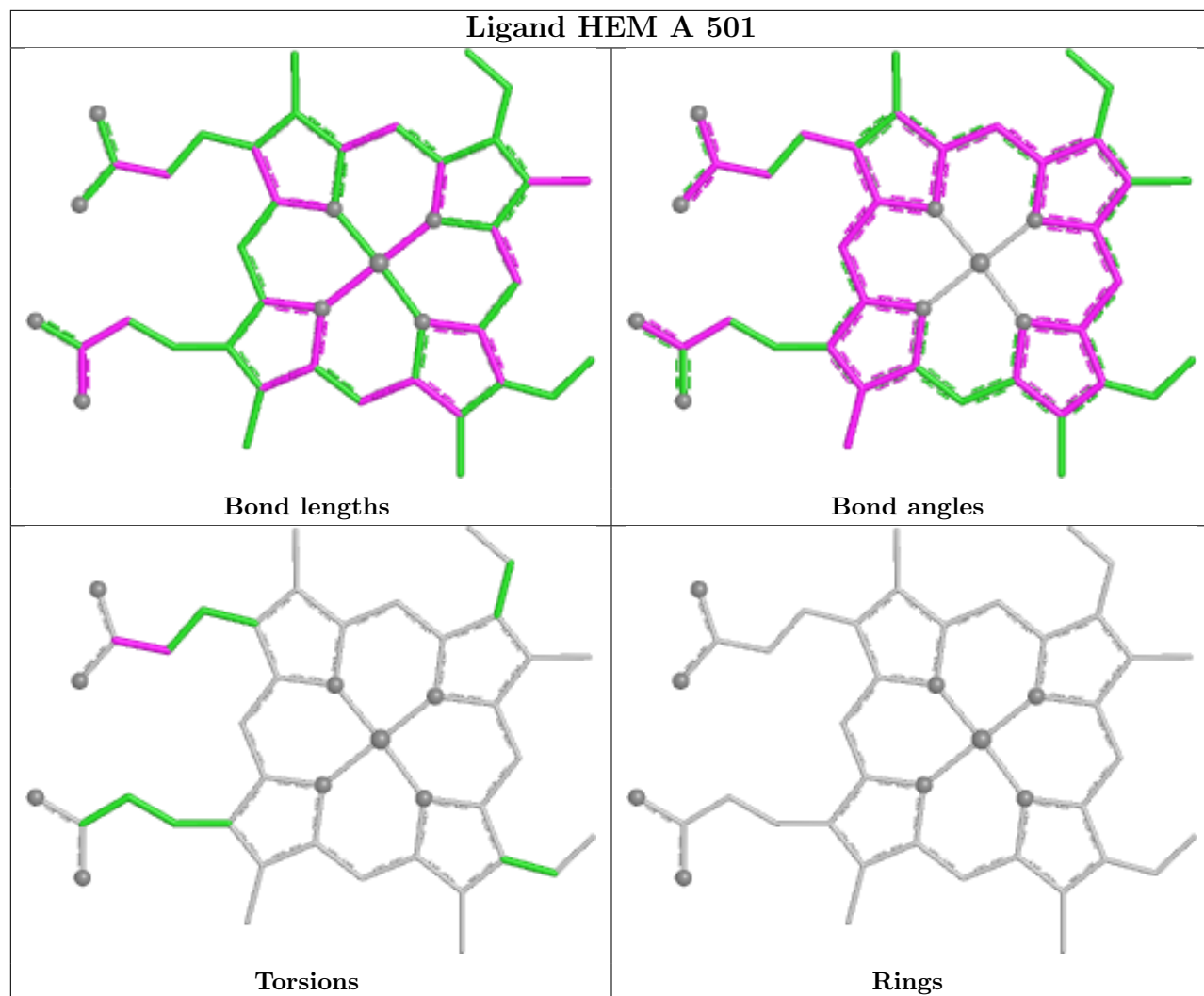
3 monomers are involved in 3 short contacts:

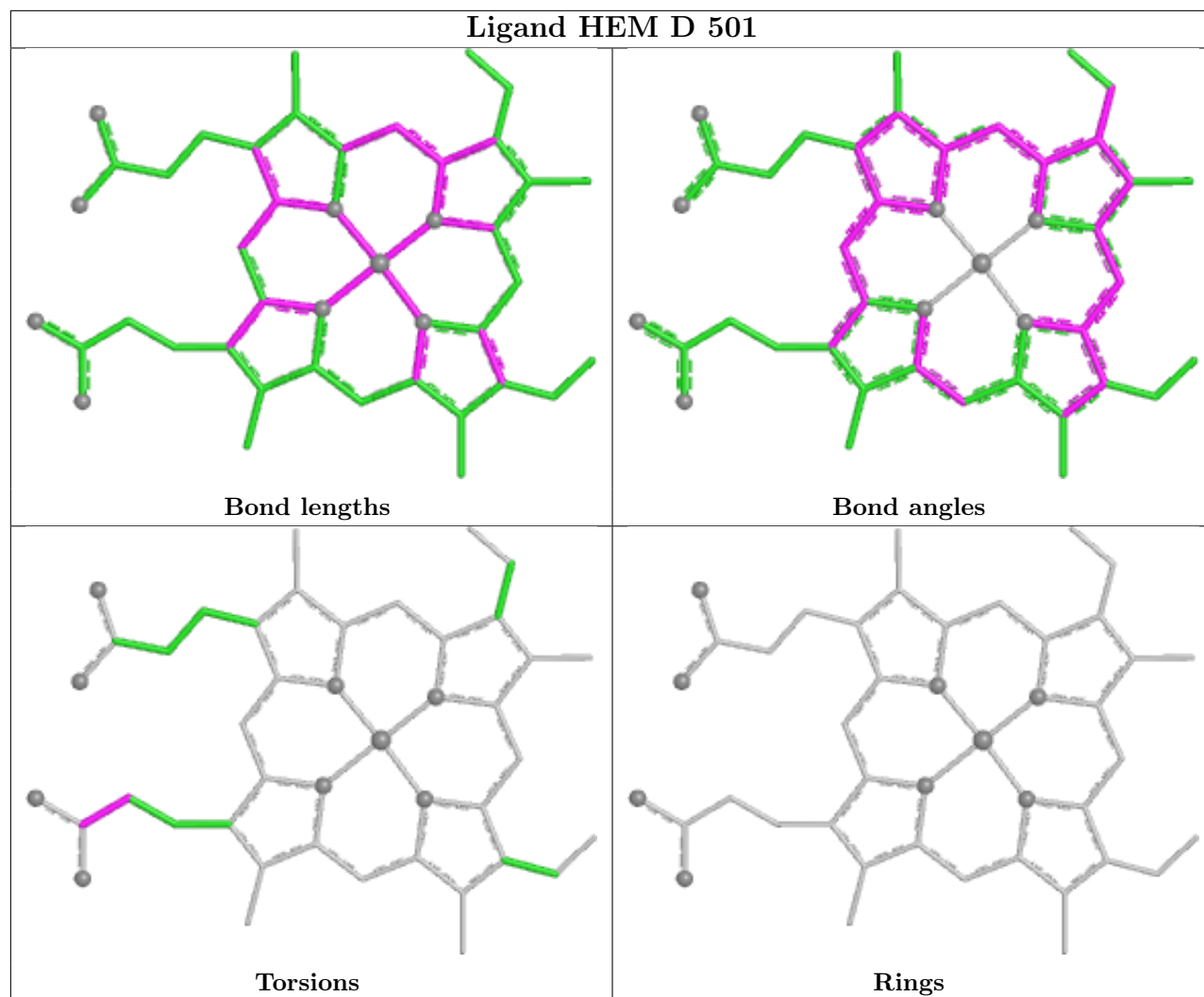
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	A1L3V	1	0
2	A	501	HEM	1	0
3	D	502	A1L3V	1	0

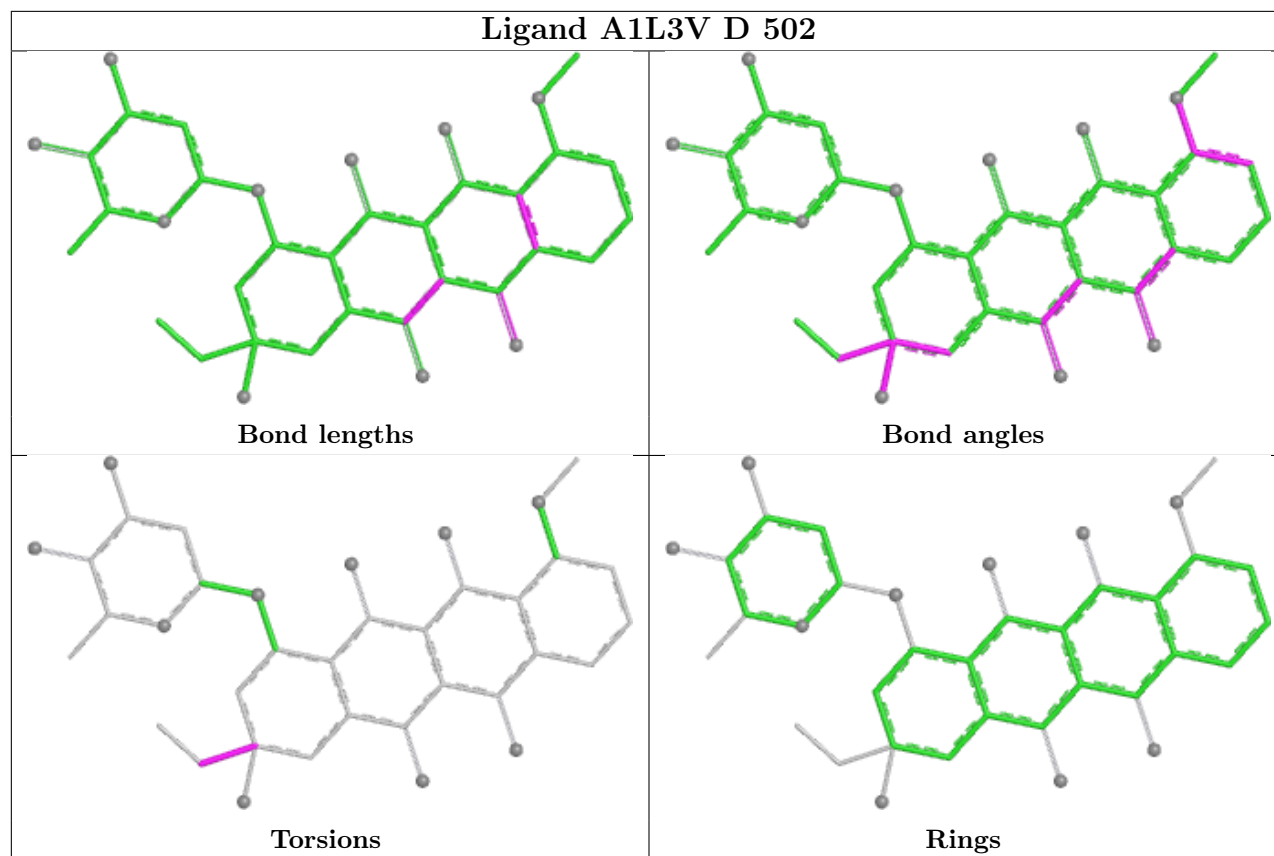
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand A1L3V A 502









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	406/457 (88%)	0.43	24 (5%) 28 32	20, 35, 64, 88	0
1	D	406/457 (88%)	0.62	20 (4%) 35 40	23, 39, 65, 84	0
All	All	812/914 (88%)	0.53	44 (5%) 31 35	20, 37, 65, 88	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	207	PRO	8.1
1	D	192	PRO	5.7
1	A	357	TRP	5.7
1	D	207	PRO	5.4
1	D	78	GLY	4.1
1	A	319	ILE	3.8
1	D	191	GLY	3.7
1	A	81	ASP	3.6
1	D	3	GLY	3.6
1	D	79	VAL	3.4
1	A	230	THR	3.3
1	D	228	THR	3.3
1	A	192	PRO	3.3
1	A	79	VAL	3.3
1	A	228	THR	3.2
1	D	229	PRO	3.2
1	A	229	PRO	3.1
1	D	81	ASP	3.0
1	A	284	ALA	2.9
1	D	357	TRP	2.9
1	A	320	GLY	2.9
1	D	80	ASP	2.9
1	D	397	VAL	2.8
1	D	319	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	355	PRO	2.7
1	A	358	ARG	2.7
1	A	407	LYS	2.7
1	A	225	ARG	2.6
1	A	4	GLU	2.6
1	D	74	ALA	2.6
1	A	191	GLY	2.5
1	D	321	GLY	2.5
1	A	321	GLY	2.4
1	D	75	ALA	2.4
1	A	78	GLY	2.3
1	A	75	ALA	2.2
1	A	234	VAL	2.1
1	D	284	ALA	2.1
1	D	227	ASP	2.1
1	A	74	ALA	2.1
1	D	9	ALA	2.1
1	D	322	VAL	2.1
1	A	80	ASP	2.1
1	A	118	ARG	2.1

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.

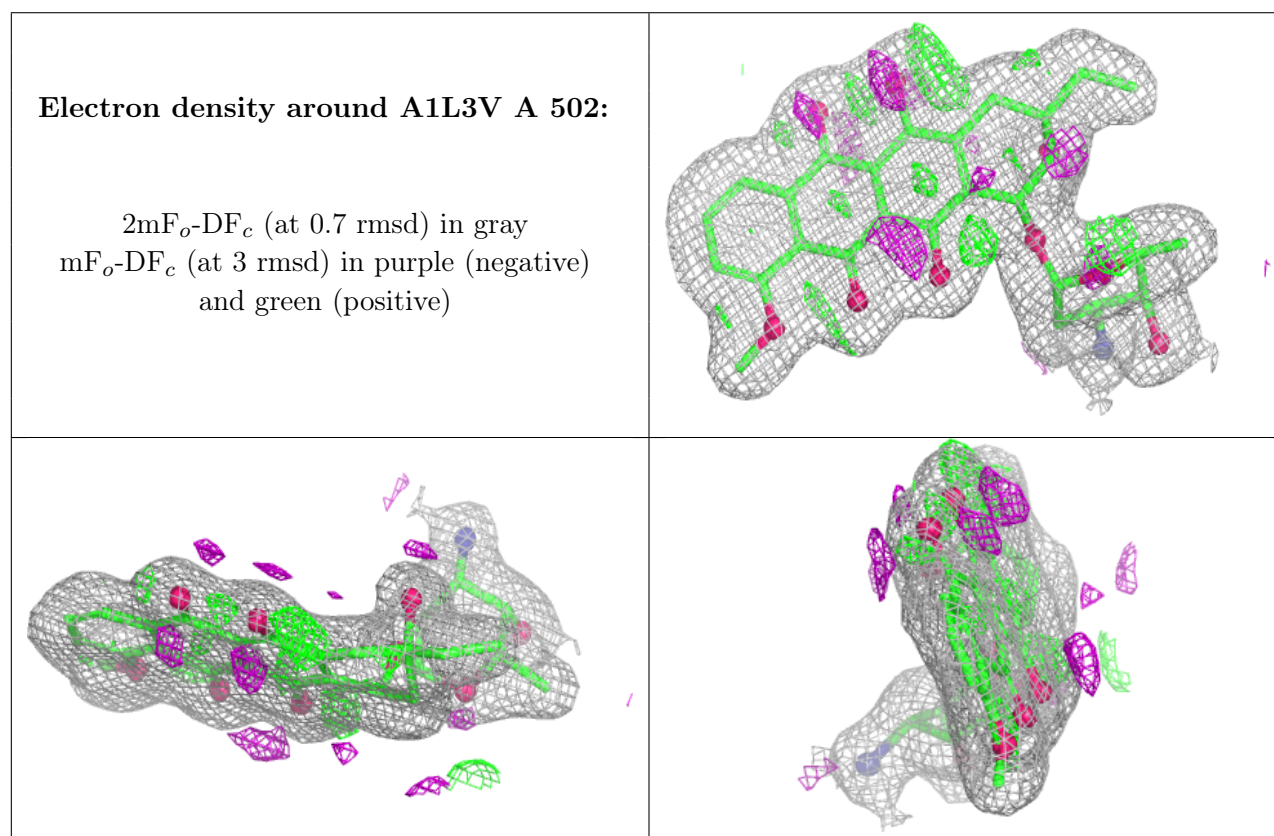
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	A1L3V	A	502	37/37	0.93	0.09	18,23,27,28	0
3	A1L3V	D	502	37/37	0.94	0.08	24,28,34,35	0
2	HEM	A	501	43/43	0.96	0.08	15,21,26,30	0

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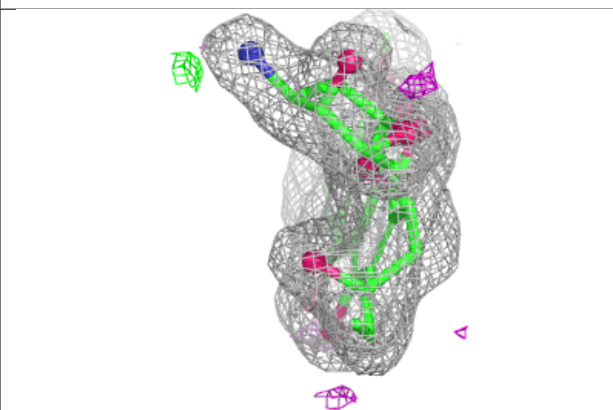
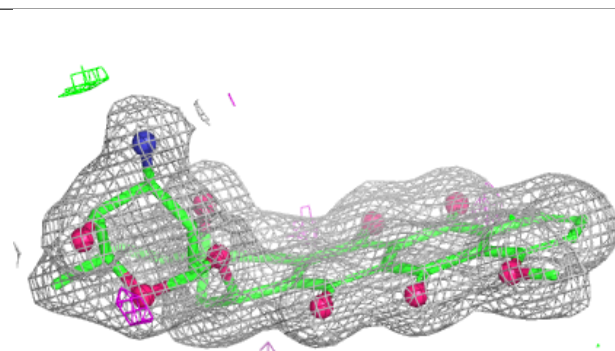
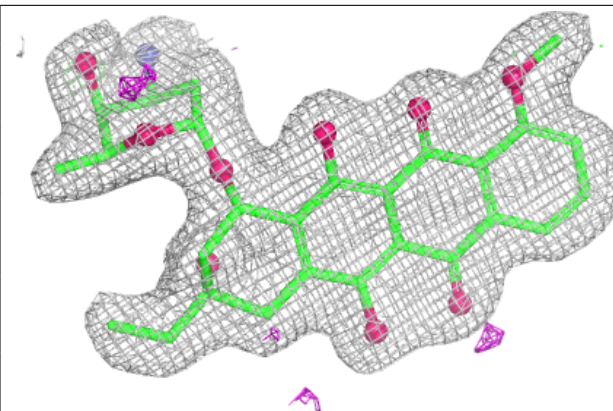
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	D	501	43/43	0.97	0.07	18,23,30,35	0

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



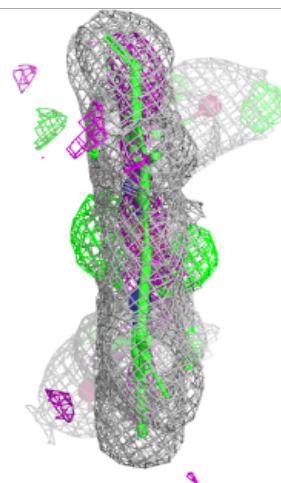
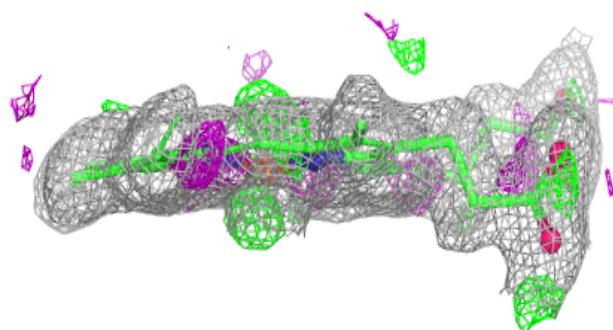
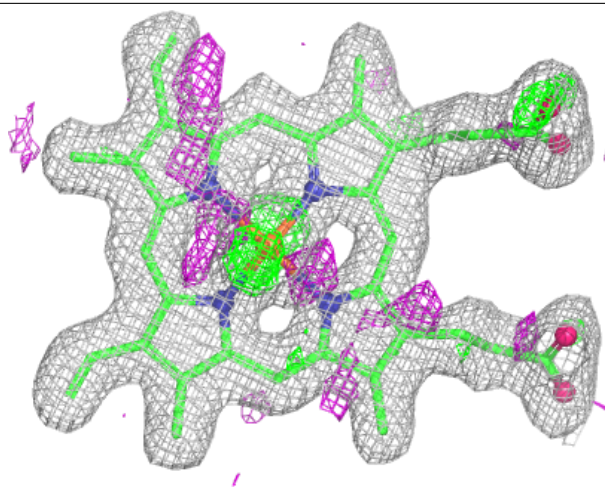
Electron density around A1L3V D 502:

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



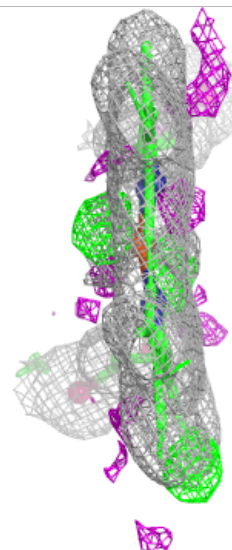
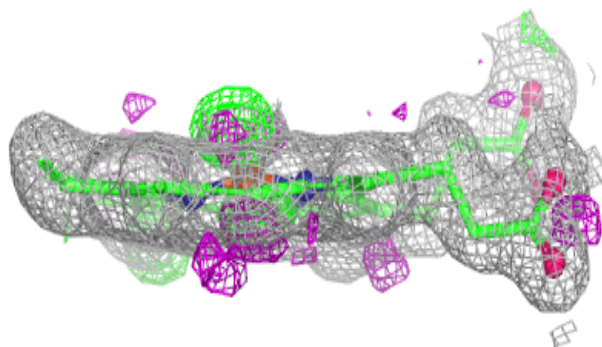
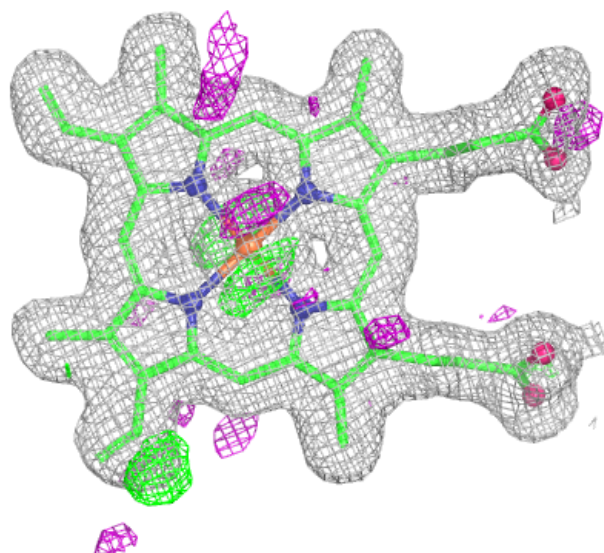
Electron density around HEM A 501:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.