



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 11:10 AM EDT

PDB ID : 8D8P
Title : Crystal structure of a novel fatty acid decarboxylase from *Rothia nasimurium*
Authors : Vieira, P.S.; Murakami, M.T.; Zaphorlin, L.M.
Deposited on : 2022-06-08
Resolution : 2.75 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

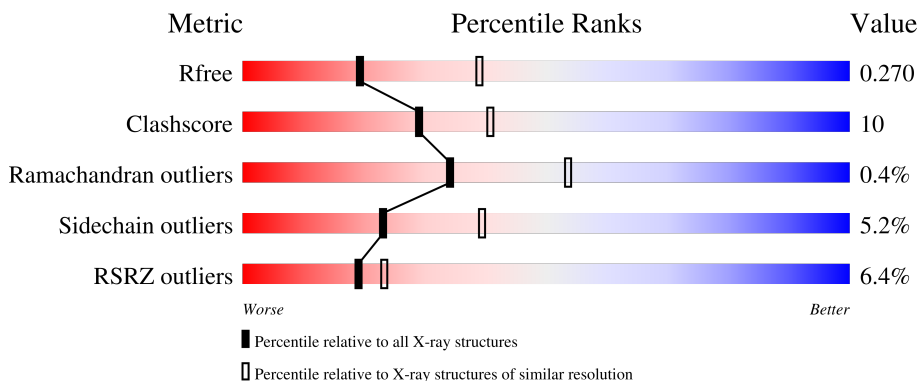
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

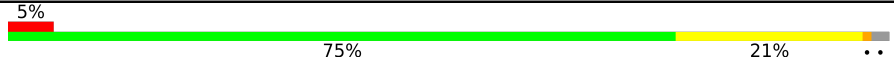

The reported resolution of this entry is 2.75 Å.

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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	429	
1	B	429	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6721 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 Decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	420	Total 3257	C 2043	N 580	O 619	S 15	0	0	0
1	B	420	Total 3257	C 2043	N 580	O 619	S 15	0	0	0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			18	16	2		
3	B	1	Total	C	O	0	0
			18	16	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

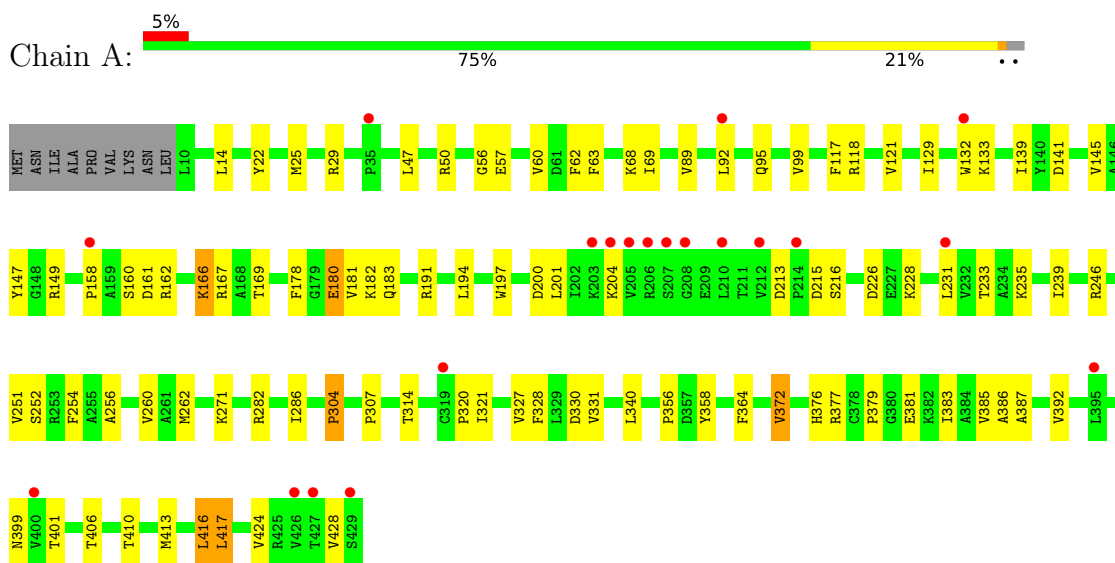
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	17	Total	O	0	0
			17	17		
5	B	8	Total	O	0	0
			8	8		

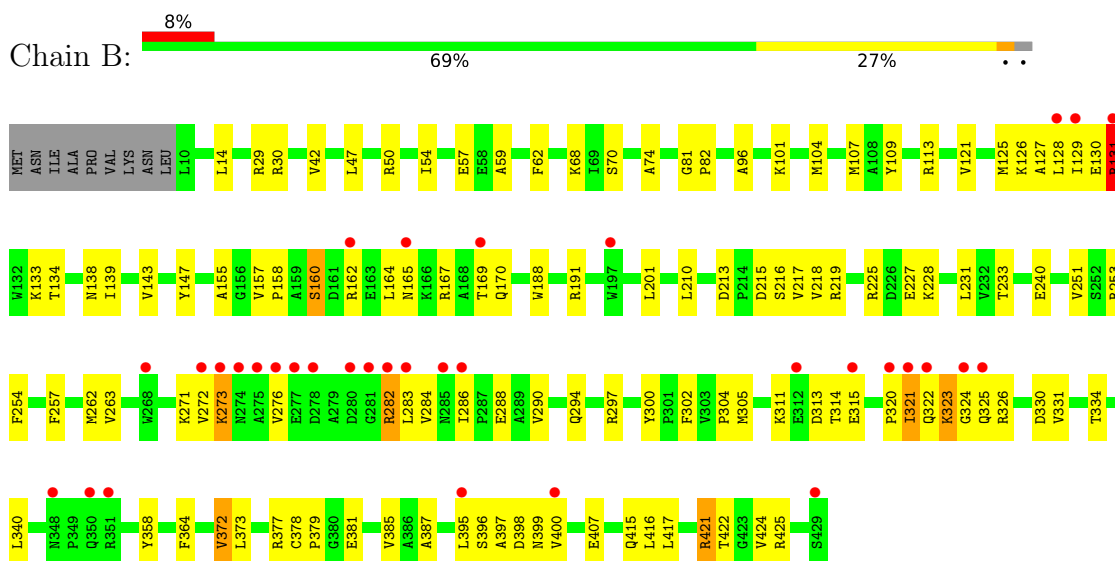
3 Residue-property plots [i](#)

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: Decarboxylase



- Molecule 1: Decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	57.55Å 203.38Å 316.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.41 – 2.75 49.02 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.41-2.75) 99.9 (49.02-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.77Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.228 , 0.269 0.230 , 0.270	Depositor DCC
R_{free} test set	1226 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	74.4	Xtrriage
Anisotropy	0.133	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6721	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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: SO4, HEM, PLM

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	0.28	0/3323	0.52	2/4504 (0.0%)
1	B	0.31	1/3323 (0.0%)	0.59	6/4504 (0.1%)
All	All	0.29	1/6646 (0.0%)	0.56	8/9008 (0.1%)

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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	273	LYS	CB-CG	-5.25	1.38	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	273	LYS	CD-CE-NZ	11.53	138.22	111.70
1	B	131	ARG	CG-CD-NE	-8.90	93.10	111.80
1	B	131	ARG	N-CA-CB	-6.44	99.02	110.60
1	A	271	LYS	CB-CG-CD	5.50	125.91	111.60
1	B	321	ILE	C-N-CA	5.42	135.25	121.70
1	B	131	ARG	CB-CA-C	5.37	121.15	110.40
1	B	131	ARG	CA-CB-CG	5.26	124.97	113.40
1	A	166	LYS	CB-CG-CD	5.01	124.64	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	131	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3257	0	3218	53	0
1	B	3257	0	3218	73	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
3	A	18	0	31	4	0
3	B	18	0	31	3	0
4	A	30	0	0	0	0
4	B	30	0	0	0	0
5	A	17	0	0	0	0
5	B	8	0	0	0	0
All	All	6721	0	6558	127	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 10.

All (127) 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:128:LEU:HB2	1:B:131:ARG:HH21	1.38	0.85
1:B:127:ALA:O	1:B:131:ARG:HB2	1.76	0.84
1:B:50:ARG:HD3	1:B:322:GLN:HG3	1.62	0.81
1:B:128:LEU:CB	1:B:131:ARG:HH21	2.05	0.70
1:B:128:LEU:HB2	1:B:131:ARG:NH2	2.06	0.69
1:B:273:LYS:HE3	1:B:398:ASP:OD1	1.98	0.63
1:B:50:ARG:CD	1:B:322:GLN:HG3	2.27	0.63
1:B:273:LYS:HG3	1:B:396:SER:O	1.98	0.62
1:B:130:GLU:HA	1:B:133:LYS:HD2	1.81	0.62
1:B:262:MET:HE1	1:B:395:LEU:HB2	1.82	0.61
1:A:133:LYS:HG3	1:A:428:VAL:HG13	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:THR:HG22	1:A:321:ILE:HD11	1.82	0.60
1:B:286:ILE:O	1:B:290:VAL:HG23	2.01	0.60
1:B:158:PRO:HG2	1:B:210:LEU:HD12	1.83	0.59
1:B:399:ASN:N	1:B:399:ASN:OD1	2.35	0.59
1:B:213:ASP:HB3	1:B:216:SER:HB3	1.84	0.59
1:B:304:PRO:HG2	3:B:502:PLM:HB2	1.87	0.56
1:A:307:PRO:HG3	3:A:502:PLM:HD2	1.88	0.56
1:A:262:MET:HE1	1:A:392:VAL:HA	1.87	0.55
1:B:62:PHE:CZ	1:B:321:ILE:HD11	2.42	0.55
1:B:104:MET:HE3	1:B:240:GLU:HB3	1.89	0.55
1:B:282:ARG:HD2	1:B:284:VAL:O	2.06	0.54
1:B:330:ASP:O	1:B:334:THR:HG23	2.06	0.54
1:A:50:ARG:NH2	1:A:320:PRO:O	2.41	0.53
1:B:271:LYS:O	1:B:271:LYS:HD2	2.07	0.53
1:B:101:LYS:HE3	1:B:379:PRO:HD3	1.91	0.53
1:B:139:ILE:O	1:B:143:VAL:HB	2.09	0.52
1:A:282:ARG:O	1:A:286:ILE:HD11	2.10	0.52
1:B:294:GLN:NE2	1:B:385:VAL:HG21	2.25	0.52
1:B:121:VAL:HG21	1:B:387:ALA:HA	1.92	0.51
1:B:297:ARG:NH2	1:B:381:GLU:OE2	2.44	0.51
1:A:29:ARG:NH2	1:A:330:ASP:OD2	2.32	0.51
1:A:56:GLY:O	1:A:60:VAL:HG23	2.11	0.51
1:A:118:ARG:HG2	1:A:386:ALA:HB1	1.92	0.51
1:B:54:ILE:HG13	1:B:59:ALA:HB1	1.93	0.50
1:B:125:MET:HE1	1:B:143:VAL:HG22	1.93	0.50
1:B:304:PRO:HD2	3:B:502:PLM:H92	1.93	0.50
1:A:226:ASP:OD2	1:A:228:LYS:HE3	2.12	0.50
1:B:422:THR:HB	1:B:425:ARG:HG3	1.93	0.50
1:A:213:ASP:HB3	1:A:216:SER:HB3	1.94	0.49
1:B:225:ARG:HA	1:B:231:LEU:HA	1.94	0.49
1:A:62:PHE:CE2	1:A:69:ILE:HD11	2.48	0.49
1:B:407:GLU:HB3	1:B:421:ARG:HB2	1.95	0.49
1:A:376:HIS:HD1	2:A:501:HEM:CGD	2.25	0.48
1:B:50:ARG:NH2	1:B:320:PRO:O	2.46	0.48
1:B:128:LEU:HA	1:B:131:ARG:HB3	1.94	0.48
1:A:89:VAL:HA	1:A:92:LEU:HD22	1.95	0.48
1:B:57:GLU:HG3	1:B:340:LEU:HD11	1.96	0.48
1:B:311:LYS:O	1:B:323:LYS:HD2	2.13	0.48
1:A:235:LYS:O	1:A:239:ILE:HD12	2.13	0.48
1:A:158:PRO:HD2	1:A:201:LEU:HD21	1.95	0.48
1:A:381:GLU:O	1:A:385:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:THR:OG1	1:B:315:GLU:N	2.45	0.48
1:A:149:ARG:NH1	1:A:161:ASP:OD1	2.40	0.47
1:B:304:PRO:HG3	1:B:416:LEU:HD11	1.96	0.47
1:A:25:MET:SD	1:A:25:MET:N	2.88	0.46
1:B:126:LYS:HG2	1:B:283:LEU:HD11	1.98	0.46
1:A:358:TYR:HB2	1:A:364:PHE:CD2	2.51	0.46
1:A:406:THR:O	1:A:410:THR:HB	2.16	0.46
1:A:372:VAL:HA	1:A:377:ARG:HB3	1.98	0.46
1:A:356:PRO:HD2	1:B:373:LEU:HD22	1.98	0.46
1:B:372:VAL:HA	1:B:377:ARG:HB3	1.97	0.45
1:B:29:ARG:HA	1:B:42:VAL:HG21	1.98	0.45
1:A:117:PHE:CE2	1:A:383:ILE:HG23	2.52	0.45
1:B:397:ALA:HB3	1:B:400:VAL:HG12	1.98	0.45
1:B:125:MET:O	1:B:129:ILE:HG23	2.17	0.45
1:B:81:GLY:O	1:B:191:ARG:HD2	2.16	0.45
1:A:307:PRO:HA	1:A:327:VAL:O	2.16	0.45
1:B:107:MET:HE2	1:B:217:VAL:HA	1.98	0.45
3:B:502:PLM:HB1	3:B:502:PLM:HE1	1.54	0.44
1:B:253:ARG:NH1	1:B:417:LEU:O	2.51	0.44
1:A:68:LYS:HE2	1:A:314:THR:HG21	2.00	0.44
1:A:129:ILE:O	1:A:428:VAL:HG11	2.16	0.44
1:B:282:ARG:O	1:B:286:ILE:HD11	2.18	0.44
1:B:138:ASN:HA	1:B:425:ARG:HA	1.99	0.44
1:A:95:GLN:O	1:A:99:VAL:HG23	2.17	0.44
1:B:107:MET:CE	1:B:217:VAL:HA	2.48	0.44
1:B:416:LEU:HD12	1:B:416:LEU:HA	1.78	0.44
1:A:22:TYR:HB2	1:A:413:MET:HE3	1.99	0.43
1:B:322:GLN:HB2	1:B:325:GLN:HB2	1.99	0.43
1:B:323:LYS:HG3	1:B:324:GLY:N	2.33	0.43
1:B:165:ASN:O	1:B:169:THR:HG23	2.18	0.43
1:A:132:TRP:CH2	1:A:139:ILE:HD13	2.54	0.43
1:A:304:PRO:HD2	3:A:502:PLM:H81	1.99	0.43
1:A:321:ILE:HD12	1:A:321:ILE:O	2.17	0.43
1:A:121:VAL:HG21	1:A:387:ALA:HA	1.99	0.43
1:A:256:ALA:O	1:A:260:VAL:HG23	2.19	0.43
1:B:272:VAL:O	1:B:276:VAL:HG12	2.18	0.43
1:B:378:CYS:HB2	2:B:501:HEM:C1A	2.53	0.43
1:B:82:PRO:HD3	1:B:188:TRP:CZ2	2.54	0.43
1:B:271:LYS:HG3	1:B:288:GLU:HG2	2.00	0.43
1:B:147:TYR:CE1	1:B:387:ALA:HB1	2.53	0.42
1:A:399:ASN:OD1	1:A:399:ASN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ALA:HA	1:B:227:GLU:HB3	2.01	0.42
1:B:157:VAL:HG13	1:B:201:LEU:HD21	2.02	0.42
1:A:167:ARG:HG3	1:A:197:TRP:CE3	2.54	0.42
1:B:14:LEU:HD22	1:B:47:LEU:HD23	2.01	0.42
1:B:167:ARG:NH1	1:B:170:GLN:OE1	2.44	0.42
1:B:251:VAL:HA	2:B:501:HEM:HBB1	2.01	0.42
1:B:271:LYS:HE2	1:B:288:GLU:HG2	2.02	0.42
1:B:313:ASP:OD1	1:B:323:LYS:N	2.52	0.42
1:B:126:LYS:O	1:B:129:ILE:HG12	2.19	0.42
3:A:502:PLM:HE1	3:A:502:PLM:HB1	1.49	0.42
1:A:57:GLU:HG3	1:A:340:LEU:HD21	2.01	0.42
1:A:181:VAL:HG23	1:A:182:LYS:HG3	2.02	0.42
1:B:155:ALA:O	1:B:218:VAL:HG23	2.19	0.42
1:A:132:TRP:HH2	1:A:139:ILE:HD13	1.85	0.41
1:A:417:LEU:HD22	1:A:417:LEU:HA	1.86	0.41
1:B:107:MET:HA	1:B:113:ARG:HD3	2.02	0.41
1:B:160:SER:O	1:B:164:LEU:HG	2.19	0.41
1:A:246:ARG:HH21	3:A:502:PLM:C1	2.33	0.41
1:A:180:GLU:HB3	1:A:183:GLN:HB2	2.02	0.41
1:A:379:PRO:HD2	2:A:501:HEM:C1D	2.55	0.41
1:A:14:LEU:HD22	1:A:47:LEU:HD23	2.02	0.41
1:A:63:PHE:HA	1:A:69:ILE:HD13	2.02	0.41
1:A:416:LEU:HD22	1:A:416:LEU:HA	1.77	0.41
1:B:257:PHE:HB3	1:B:300:TYR:CG	2.56	0.41
1:A:160:SER:OG	1:A:162:ARG:HG2	2.21	0.41
1:A:200:ASP:O	1:A:204:LYS:HG3	2.21	0.41
1:A:307:PRO:HB3	1:A:328:PHE:CE2	2.56	0.41
1:B:358:TYR:HB2	1:B:364:PHE:CD2	2.55	0.41
1:B:379:PRO:HD2	2:B:501:HEM:C2D	2.56	0.41
1:A:141:ASP:O	1:A:145:VAL:HG23	2.21	0.41
1:A:167:ARG:HD2	1:A:194:LEU:HD23	2.03	0.41
1:B:74:ALA:O	1:B:326:ARG:NH1	2.52	0.40
1:A:162:ARG:O	1:A:166:LYS:N	2.50	0.40
1:A:147:TYR:CE2	1:A:251:VAL:HB	2.57	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	418/429 (97%)	403 (96%)	13 (3%)	2 (0%)	29	47
1	B	418/429 (97%)	403 (96%)	14 (3%)	1 (0%)	47	69
All	All	836/858 (97%)	806 (96%)	27 (3%)	3 (0%)	34	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	424	VAL
1	B	424	VAL
1	A	304	PRO

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	344/352 (98%)	330 (96%)	14 (4%)	30	50
1	B	344/352 (98%)	322 (94%)	22 (6%)	17	31
All	All	688/704 (98%)	652 (95%)	36 (5%)	23	39

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	THR
1	A	178	PHE
1	A	180	GLU

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Mol	Chain	Res	Type
1	A	191	ARG
1	A	215	ASP
1	A	231	LEU
1	A	233	THR
1	A	252	SER
1	A	254	PHE
1	A	331	VAL
1	A	372	VAL
1	A	401	THR
1	A	416	LEU
1	A	417	LEU
1	B	30	ARG
1	B	68	LYS
1	B	70	SER
1	B	109	TYR
1	B	131	ARG
1	B	134	THR
1	B	160	SER
1	B	162	ARG
1	B	215	ASP
1	B	219	ARG
1	B	228	LYS
1	B	233	THR
1	B	254	PHE
1	B	263	VAL
1	B	282	ARG
1	B	302	PHE
1	B	305	MET
1	B	323	LYS
1	B	331	VAL
1	B	372	VAL
1	B	415	GLN
1	B	421	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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
4	SO4	B	507	-	4,4,4	0.15	0	6,6,6	0.05	0
4	SO4	A	504	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	A	508	-	4,4,4	0.14	0	6,6,6	0.05	0
2	HEM	B	501	1	41,50,50	1.50	5 (12%)	45,82,82	1.51	8 (17%)
4	SO4	A	507	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	B	503	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	B	508	-	4,4,4	0.14	0	6,6,6	0.05	0
2	HEM	A	501	1	41,50,50	1.49	5 (12%)	45,82,82	1.47	8 (17%)
4	SO4	B	504	-	4,4,4	0.13	0	6,6,6	0.06	0
4	SO4	A	505	-	4,4,4	0.14	0	6,6,6	0.05	0
3	PLM	B	502	-	17,17,17	0.85	1 (5%)	17,17,17	0.75	2 (11%)
3	PLM	A	502	-	17,17,17	0.89	1 (5%)	17,17,17	0.78	2 (11%)
4	SO4	B	506	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	506	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	A	503	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	B	505	-	4,4,4	0.14	0	6,6,6	0.06	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	501	1	-	4/12/54/54	-
3	PLM	B	502	-	-	9/15/15/15	-
2	HEM	A	501	1	-	4/12/54/54	-
3	PLM	A	502	-	-	9/15/15/15	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3C-C2C	-4.34	1.34	1.40
2	A	501	HEM	C3C-C2C	-4.25	1.34	1.40
2	A	501	HEM	C3C-CAC	3.68	1.55	1.47
2	B	501	HEM	C3C-CAC	3.66	1.55	1.47
2	B	501	HEM	CAB-C3B	2.81	1.55	1.47
2	A	501	HEM	CAB-C3B	2.79	1.55	1.47
3	A	502	PLM	C2-C1	2.78	1.57	1.50
3	B	502	PLM	C2-C1	2.69	1.56	1.50
2	A	501	HEM	CMD-C2D	2.03	1.55	1.50
2	A	501	HEM	CMB-C2B	2.02	1.55	1.50
2	B	501	HEM	CMD-C2D	2.02	1.55	1.50
2	B	501	HEM	CMB-C2B	2.01	1.55	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	C4D-ND-C1D	2.89	108.05	105.07
2	A	501	HEM	C4D-ND-C1D	2.84	108.01	105.07
2	B	501	HEM	C1B-NB-C4B	2.83	108.00	105.07
2	A	501	HEM	CAD-CBD-CGD	-2.79	107.60	113.60
2	A	501	HEM	C1B-NB-C4B	2.77	107.93	105.07
2	B	501	HEM	C4C-CHD-C1D	2.64	126.04	122.56
2	A	501	HEM	C4B-CHC-C1C	2.59	125.97	122.56
2	B	501	HEM	C4B-CHC-C1C	2.53	125.90	122.56
2	B	501	HEM	CAD-CBD-CGD	-2.42	108.39	113.60
2	A	501	HEM	C4C-CHD-C1D	2.39	125.72	122.56
2	B	501	HEM	C3D-C4D-ND	-2.30	107.61	110.17
3	A	502	PLM	O1-C1-O2	2.26	128.92	123.30
3	B	502	PLM	O1-C1-O2	2.25	128.90	123.30
2	B	501	HEM	C3B-C2B-C1B	2.17	108.10	106.49
2	A	501	HEM	CAA-CBA-CGA	-2.12	107.80	113.76
2	A	501	HEM	C3D-C4D-ND	-2.12	107.81	110.17
2	A	501	HEM	C3B-C2B-C1B	2.10	108.05	106.49
3	A	502	PLM	O2-C1-C2	-2.07	116.44	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	CAA-CBA-CGA	-2.06	107.99	113.76
3	B	502	PLM	O2-C1-C2	-2.03	116.57	123.08

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	HEM	C2B-C3B-CAB-CBB
2	B	501	HEM	C2B-C3B-CAB-CBB
3	A	502	PLM	CB-CC-CD-CE
3	B	502	PLM	CB-CC-CD-CE
3	A	502	PLM	CA-CB-CC-CD
3	B	502	PLM	CA-CB-CC-CD
3	A	502	PLM	C8-C9-CA-CB
3	B	502	PLM	C8-C9-CA-CB
3	B	502	PLM	C9-CA-CB-CC
3	A	502	PLM	C9-CA-CB-CC
2	A	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C4B-C3B-CAB-CBB
3	A	502	PLM	C7-C8-C9-CA
3	B	502	PLM	C7-C8-C9-CA
3	B	502	PLM	C6-C7-C8-C9
3	A	502	PLM	C6-C7-C8-C9
3	A	502	PLM	CC-CD-CE-CF
3	B	502	PLM	CC-CD-CE-CF
3	A	502	PLM	O1-C1-C2-C3
3	B	502	PLM	O1-C1-C2-C3
3	A	502	PLM	O2-C1-C2-C3
3	B	502	PLM	O2-C1-C2-C3
2	A	501	HEM	CAD-CBD-CGD-O2D
2	B	501	HEM	CAD-CBD-CGD-O2D
2	A	501	HEM	CAD-CBD-CGD-O1D
2	B	501	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

4 monomers are involved in 12 short contacts:

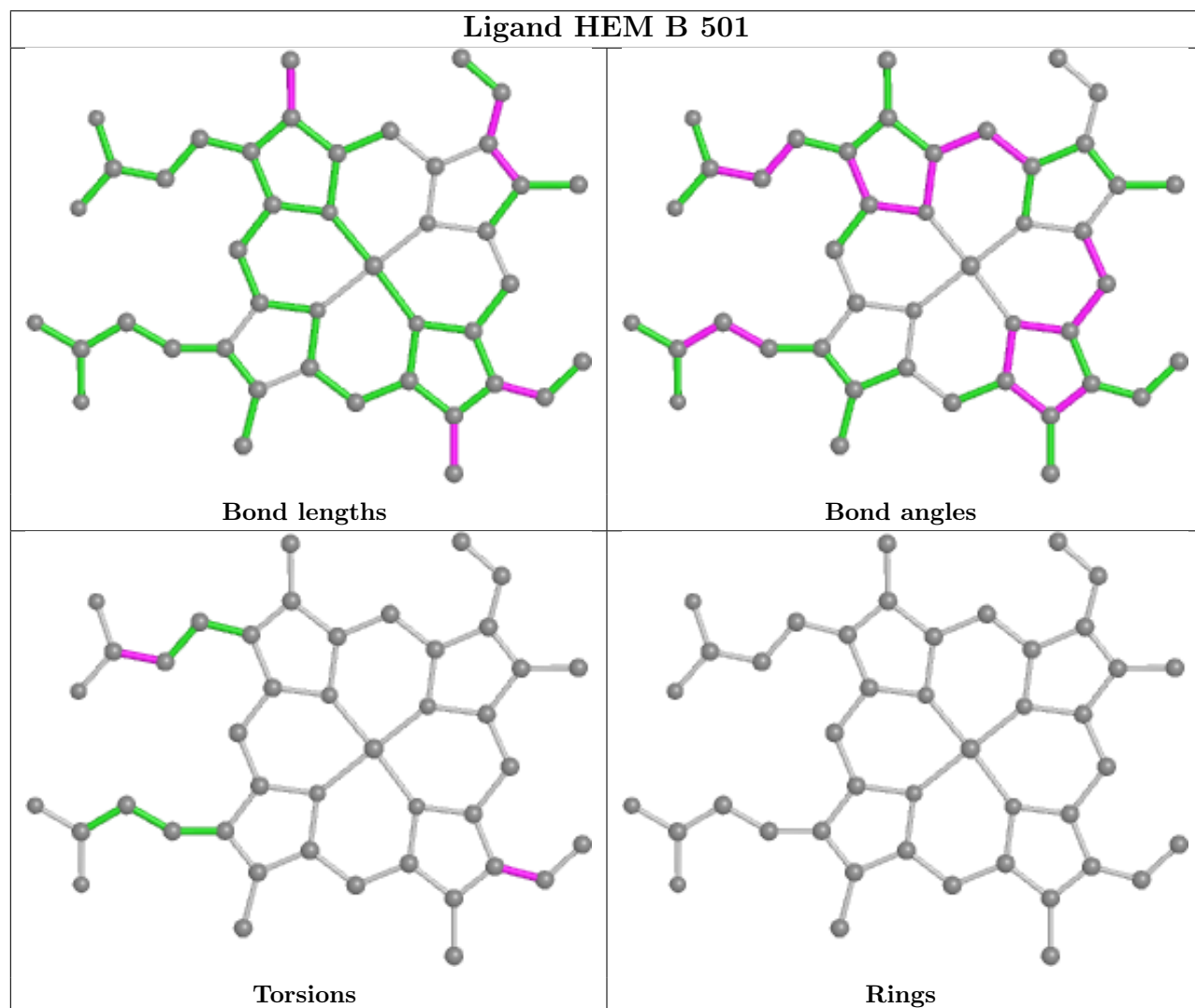
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	HEM	3	0
2	A	501	HEM	2	0
3	B	502	PLM	3	0

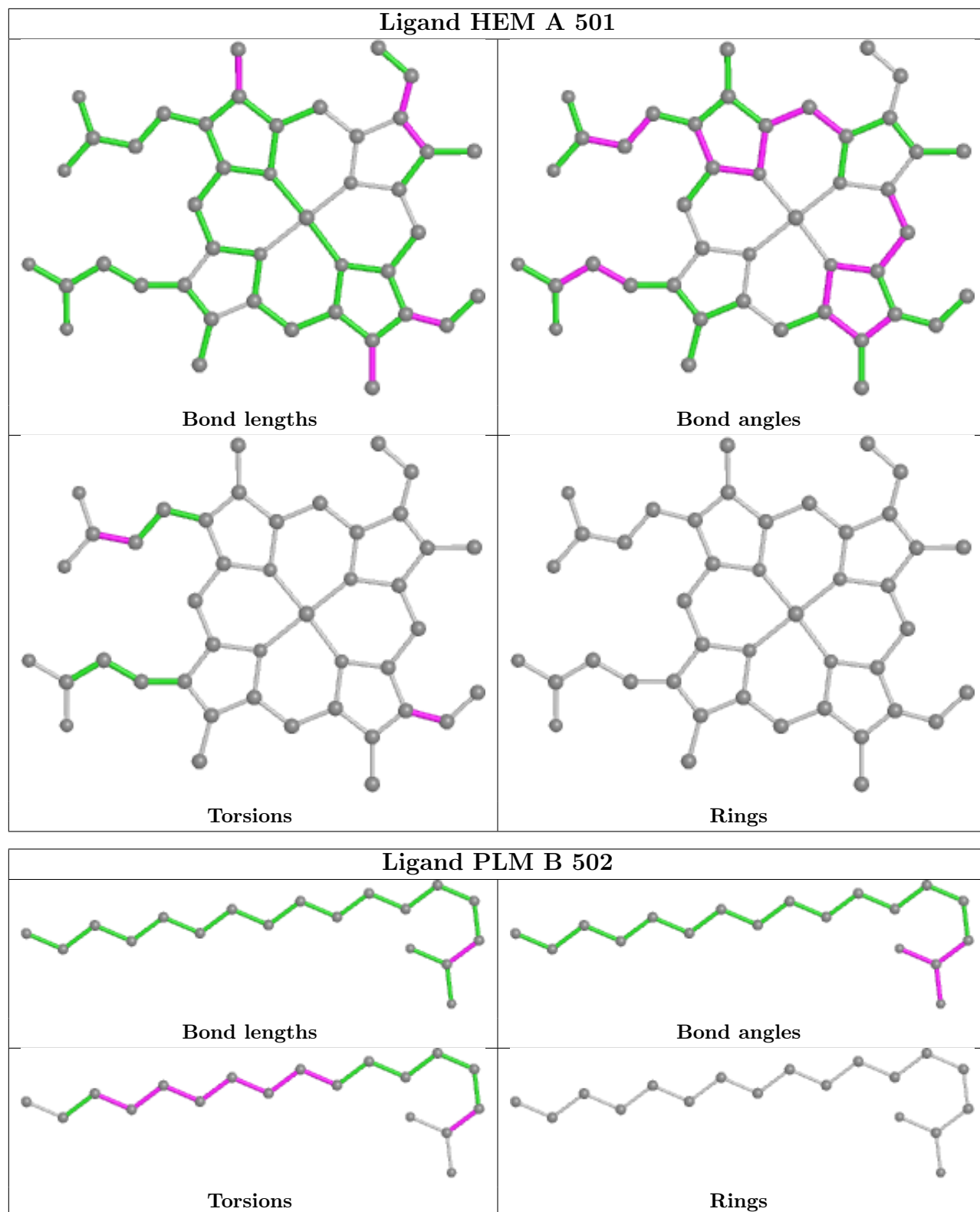
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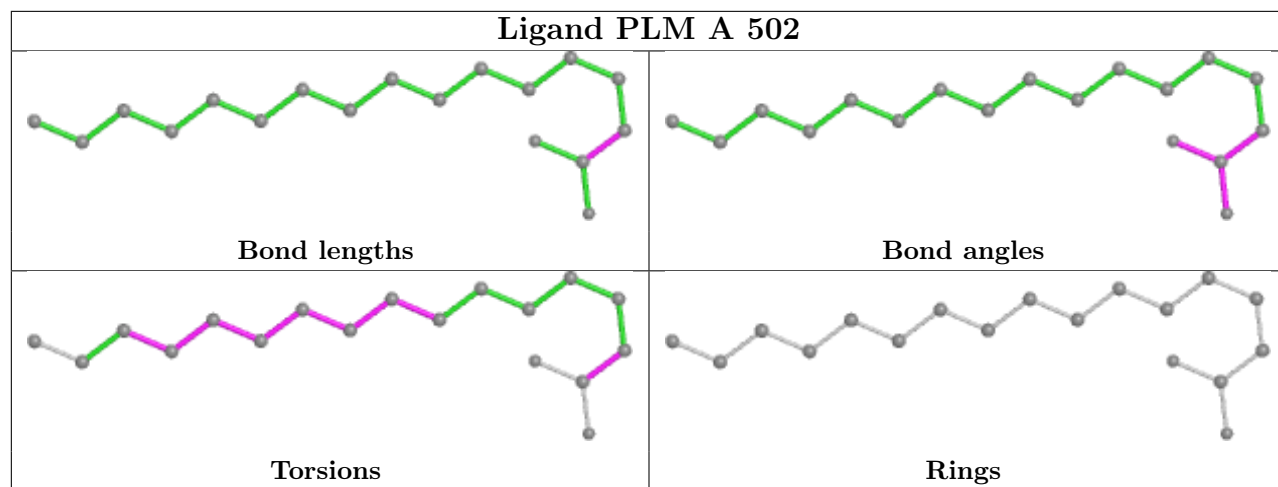
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	PLM	4	0

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	420/429 (97%)	0.41	20 (4%) 30 36	61, 74, 89, 104	0
1	B	420/429 (97%)	0.54	34 (8%) 12 14	64, 80, 104, 123	0
All	All	840/858 (97%)	0.47	54 (6%) 19 23	61, 76, 98, 123	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	281	GLY	5.2
1	B	282	ARG	4.8
1	B	272	VAL	4.5
1	B	276	VAL	4.1
1	B	280	ASP	4.0
1	B	277	GLU	4.0
1	B	324	GLY	3.9
1	B	322	GLN	3.5
1	A	210	LEU	3.5
1	A	205	VAL	3.4
1	B	429	SER	3.4
1	B	315	GLU	3.3
1	A	35	PRO	3.3
1	B	129	ILE	3.2
1	B	273	LYS	3.2
1	B	274	ASN	3.2
1	B	268	TRP	3.1
1	A	206	ARG	3.0
1	A	208	GLY	3.0
1	B	348	ASN	3.0
1	B	350	GLN	2.9
1	B	278	ASP	2.9
1	A	319	CYS	2.9
1	A	92	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	283	LEU	2.9
1	B	275	ALA	2.9
1	A	214	PRO	2.8
1	A	212	VAL	2.8
1	B	165	ASN	2.7
1	B	286	ILE	2.6
1	B	162	ARG	2.6
1	B	351	ARG	2.6
1	A	231	LEU	2.5
1	A	204	LYS	2.5
1	A	395	LEU	2.4
1	A	203	LYS	2.4
1	A	429	SER	2.3
1	A	207	SER	2.3
1	B	285	ASN	2.3
1	B	325	GLN	2.2
1	B	320	PRO	2.2
1	A	132	TRP	2.2
1	B	169	THR	2.2
1	B	321	ILE	2.2
1	A	158	PRO	2.2
1	B	131	ARG	2.2
1	A	427	THR	2.1
1	A	426	VAL	2.1
1	A	400	VAL	2.1
1	B	312	GLU	2.1
1	B	197	TRP	2.1
1	B	128	LEU	2.0
1	B	395	LEU	2.0
1	B	400	VAL	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](#)

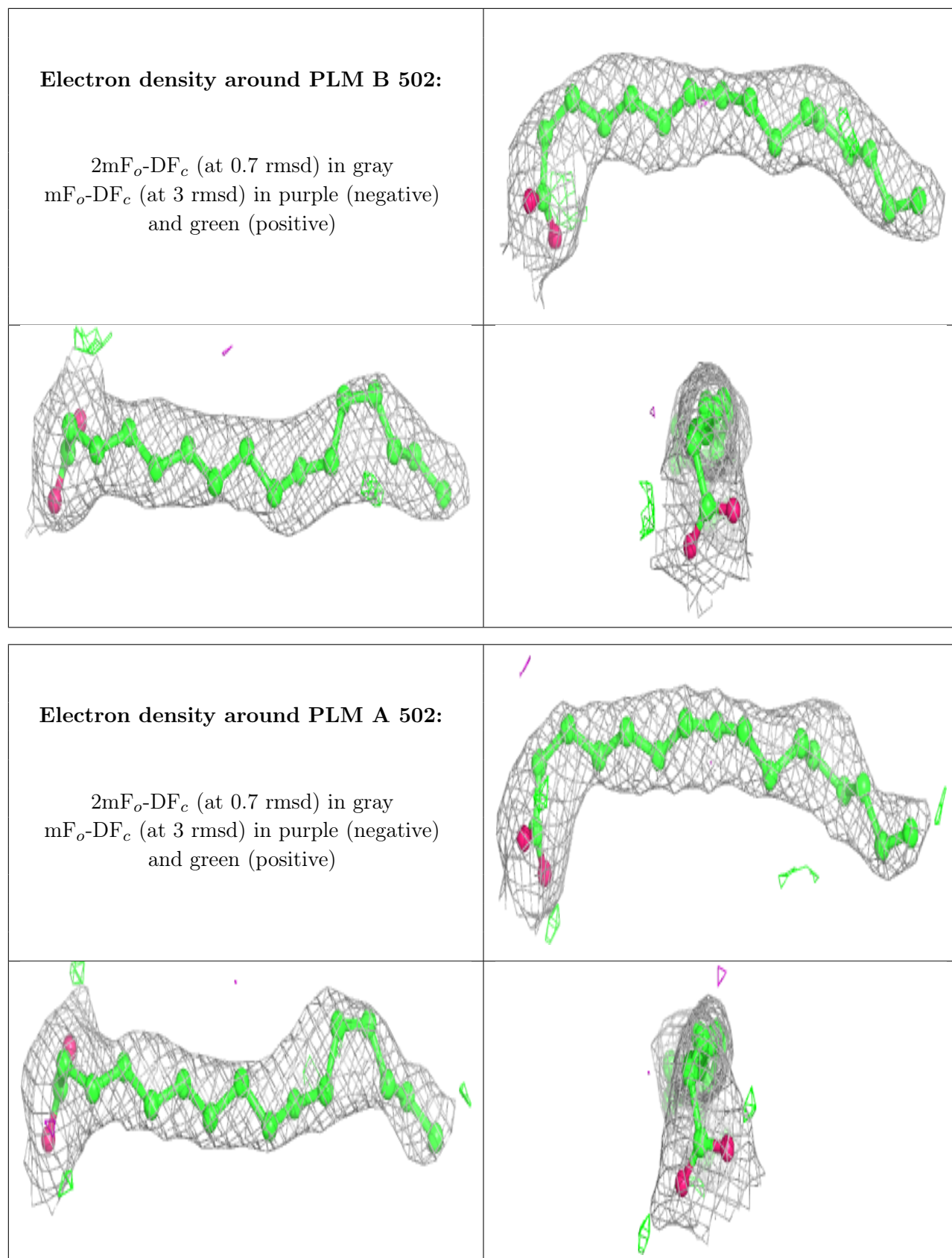
There are no monosaccharides in this entry.

6.4 Ligands

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

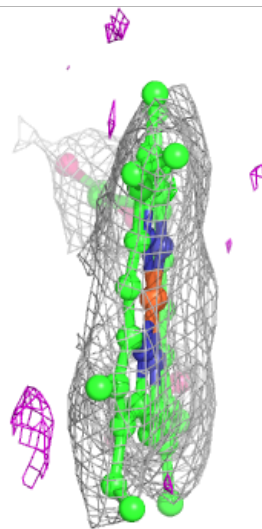
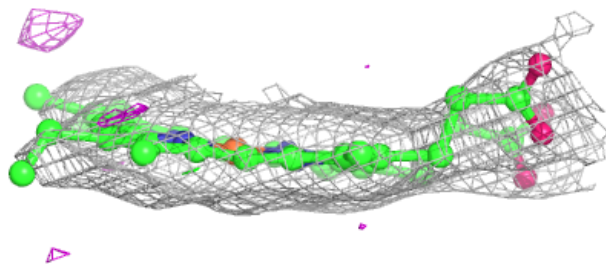
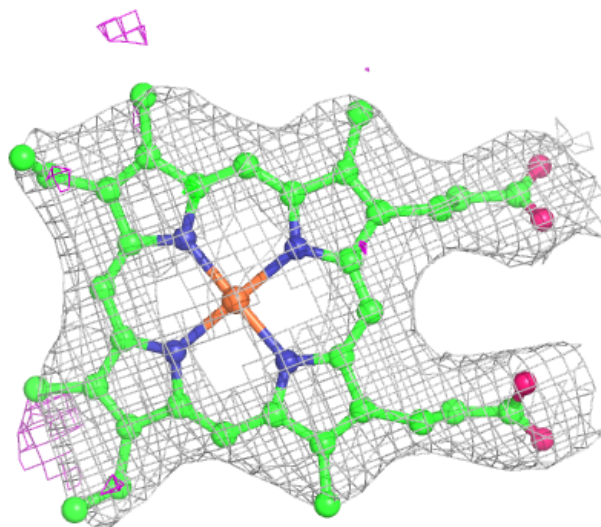
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	B	507	5/5	0.74	0.28	89,90,94,115	0
4	SO4	B	506	5/5	0.83	0.23	105,107,115,129	0
4	SO4	A	505	5/5	0.85	0.26	89,91,98,110	0
4	SO4	A	504	5/5	0.86	0.23	91,96,108,114	0
4	SO4	B	504	5/5	0.87	0.20	87,92,95,103	0
4	SO4	A	506	5/5	0.88	0.17	105,105,114,125	0
3	PLM	B	502	18/18	0.89	0.33	58,65,69,69	0
4	SO4	B	508	5/5	0.90	0.35	104,107,115,122	0
3	PLM	A	502	18/18	0.92	0.31	63,67,69,72	0
4	SO4	A	507	5/5	0.93	0.18	70,72,80,86	0
4	SO4	A	503	5/5	0.93	0.18	82,83,85,85	0
4	SO4	B	505	5/5	0.93	0.12	97,100,114,119	0
2	HEM	A	501	43/43	0.95	0.25	65,68,70,72	0
4	SO4	A	508	5/5	0.96	0.29	87,89,93,95	0
2	HEM	B	501	43/43	0.96	0.20	70,72,75,78	0
4	SO4	B	503	5/5	0.97	0.19	80,81,83,87	0

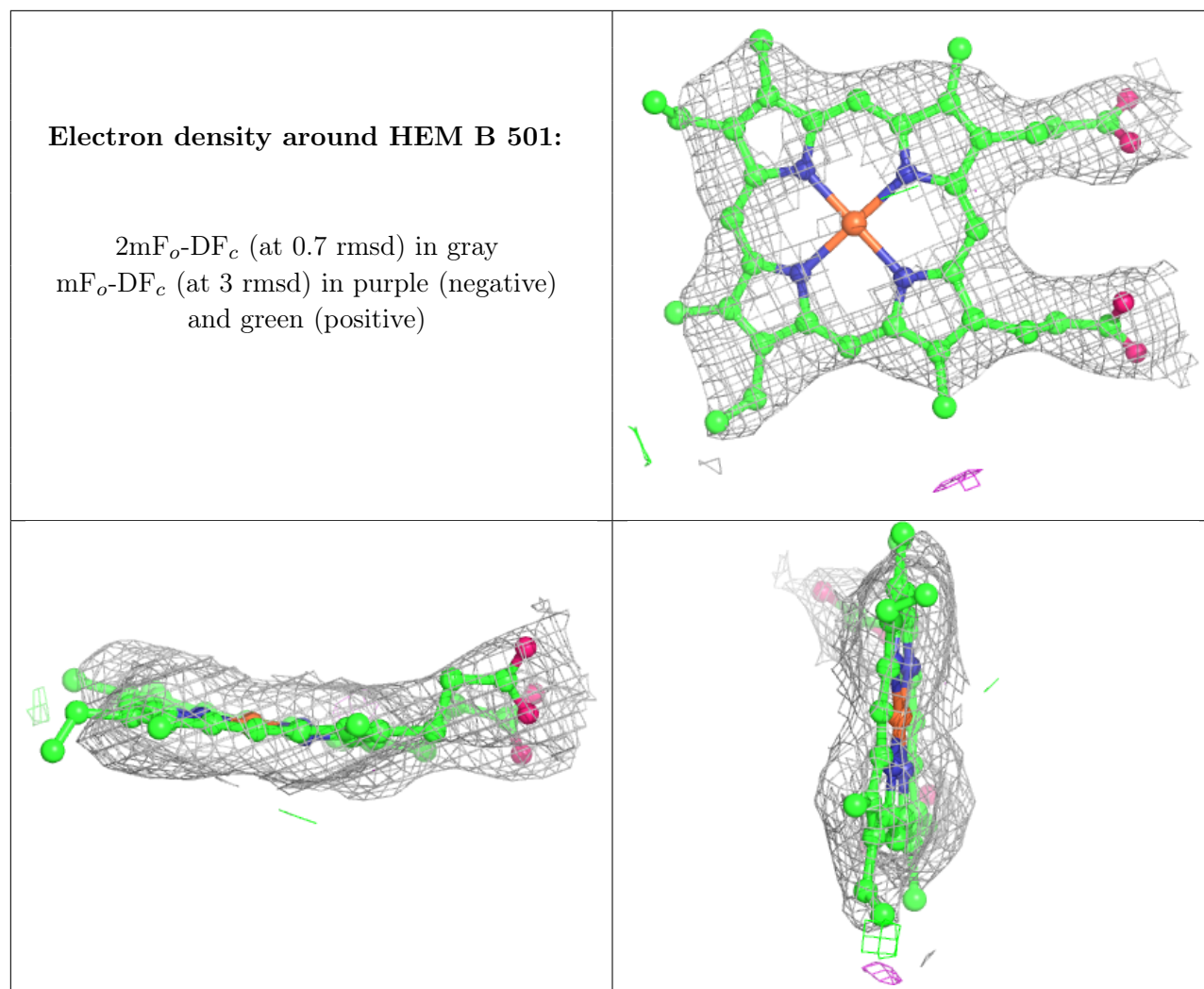
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.