Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2023 – 06:37 AM JST

PDB ID	:	6L3A
Title	:	Cytochrome P450 107G1 (RapN) with everolimus
Authors	:	Km, V.C.; Kim, D.H.; Lim, Y.R.; Lee, I.H.; Lee, J.H.; Kang, L.W.
Deposited on	:	2019-10-10
Resolution	:	3.00 Å(reported)

The following versions of software and data (see references (i)) 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 3.00 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	Percentile Ranks	Value
Rfree		0.339
Clashscore		29
Ramachandran outliers		2.5%
Sidechain outliers		14.5%
RSRZ outliers		0.5%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
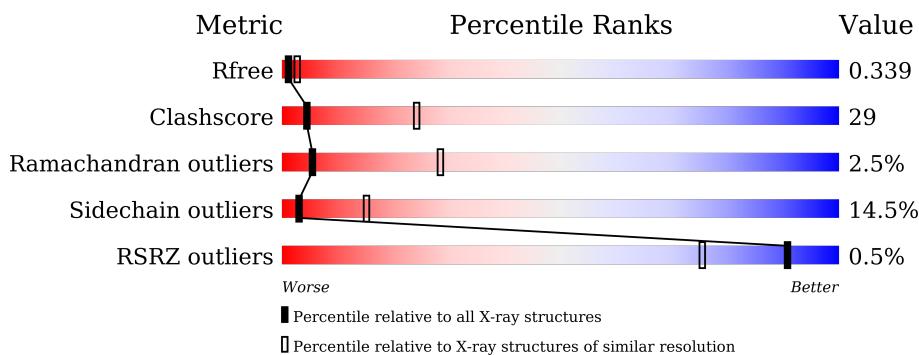
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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	404	54% 33% 9% •
1	B	404	% 56% 33% 7% •
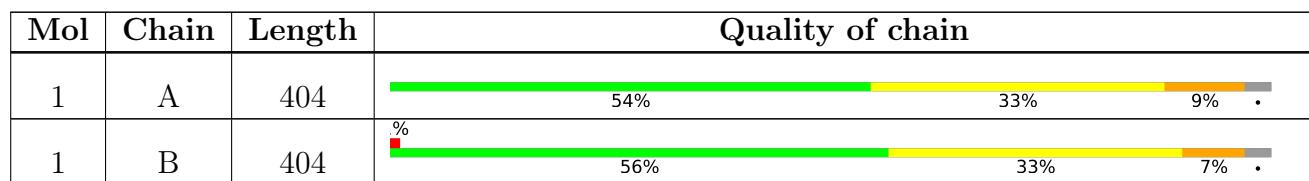
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	E53	B	502	-	-	-	X

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 6240 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 P450.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3035	1925	534	560	16			
1	B	393	Total	C	N	O	S	0	0	0
			3047	1933	534	563	17			

- 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).
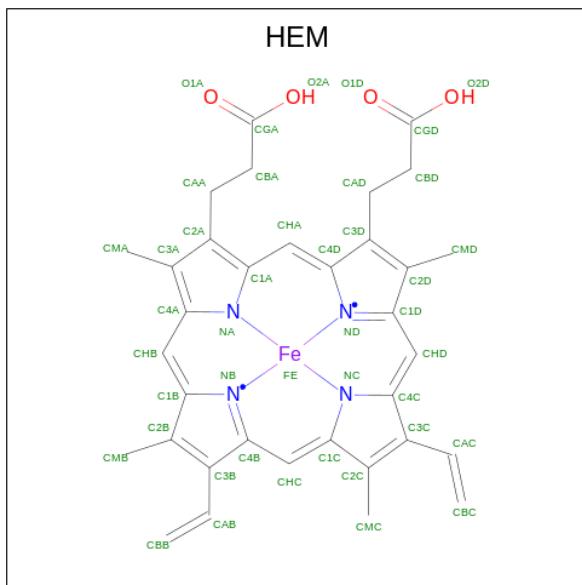
HEM

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

- Molecule 3 is Everolimus (three-letter code: E53) (formula: $C_{53}H_{83}NO_{14}$) (labeled as "Ligand of Interest" by depositor).
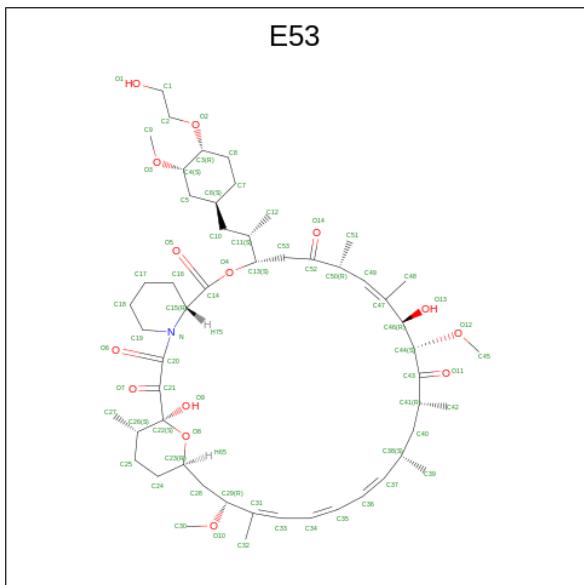
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	B	1	68	53	1	14	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	1	1	1	0	0
			Total	O		
4	B	3	3	3	0	0

3　Residue-property plots ⓘ

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: Cytochrome P450

Chain A:

- Molecule 1: Cytochrome P450

Chain B:

R373 I374 P375 A376 L377 R378 F379 A380 V381 P382 E383 P384 R385 I386 L389 R390 V394 P395 S396 L400 P401 L402 T403 W404
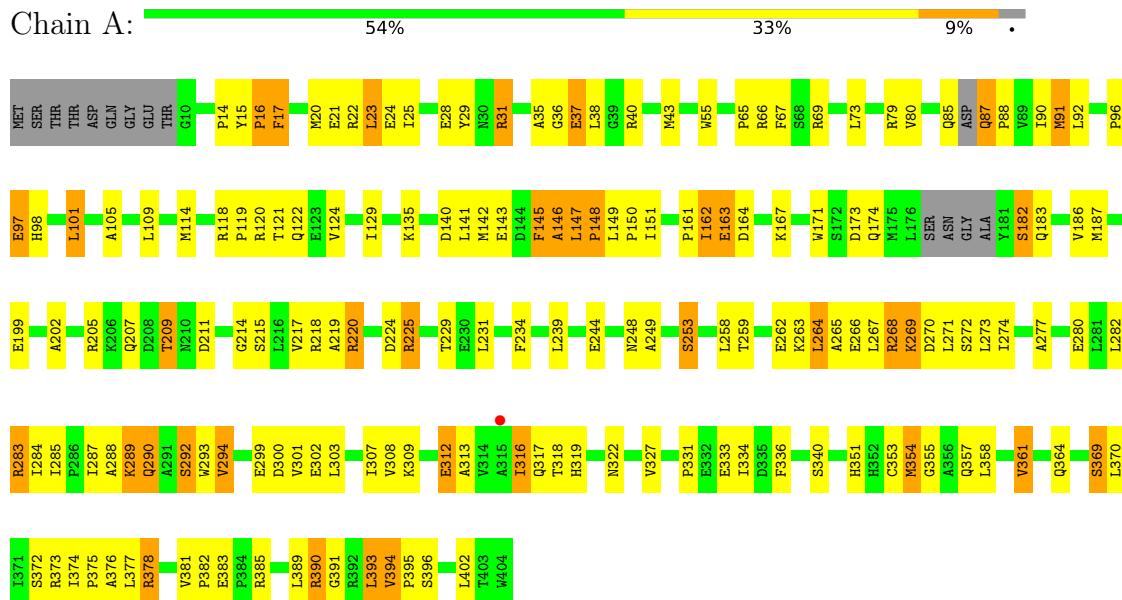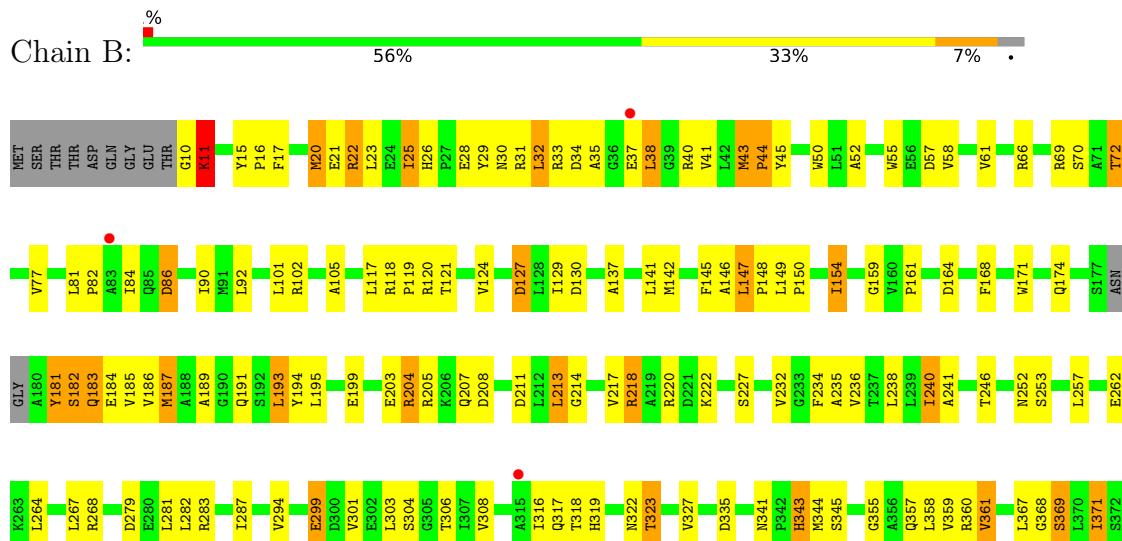
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.03Å　126.14Å　70.10Å 90.00°　116.46°　90.00°	Depositor
Resolution (Å)	44.49　–　3.00 44.49　–　3.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (44.49-3.00) 97.6 (44.49-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.58 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.241　,　0.336 0.253　,　0.339	Depositor DCC
R_{free} test set	1055 reflections (5.42%)	wwPDB-VP
Wilson B-factor (Å^2)	69.7	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.4	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.217 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6240	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, E53

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	0.69	0/3095	0.87	1/4205 (0.0%)
1	B	0.68	0/3109	0.85	1/4227 (0.0%)
All	All	0.68	0/6204	0.86	2/8432 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	146	ALA	O-C-N	6.08	132.43	122.70
1	B	213	LEU	C-N-CA	-5.32	111.12	122.30

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3035	0	3062	183	0
1	B	3047	0	3067	165	0
2	A	43	0	30	7	0
2	B	43	0	30	7	0
3	B	68	0	0	3	0
4	A	1	0	0	0	0
4	B	3	0	0	1	0

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6240	0	6189	356	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 29.

All (356) 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:162:ILE:HD13	1:A:163:GLU:N	1.26	1.42
1:A:287:ILE:O	1:A:394:VAL:CG1	1.69	1.39
1:B:15:TYR:HD2	1:B:43:MET:CE	1.41	1.32
1:B:28:GLU:O	1:B:32:LEU:HD11	1.21	1.30
1:B:28:GLU:O	1:B:32:LEU:CD1	1.79	1.30
1:B:182:SER:O	1:B:184:GLU:N	1.66	1.27
1:A:15:TYR:O	1:A:17:PHE:HD1	1.13	1.26
1:A:15:TYR:O	1:A:17:PHE:CD1	1.90	1.25
1:A:162:ILE:CD1	1:A:163:GLU:H	1.49	1.24
1:B:45:TYR:CE2	1:B:82:PRO:N	2.07	1.22
1:A:265:ALA:O	1:A:269:LYS:HG3	1.36	1.20
1:A:287:ILE:O	1:A:394:VAL:HG13	1.04	1.18
1:B:15:TYR:CD2	1:B:43:MET:CE	2.27	1.18
1:B:45:TYR:HE2	1:B:82:PRO:N	1.39	1.16
1:A:290:GLN:NE2	1:A:393:LEU:O	1.84	1.11
1:A:220:ARG:HD3	1:A:225:ARG:HG3	1.25	1.11
1:B:15:TYR:CD2	1:B:43:MET:HE3	1.85	1.10
1:B:84:ILE:O	1:B:86:ASP:OD1	1.69	1.09
1:B:45:TYR:HE2	1:B:82:PRO:CD	1.67	1.07
1:A:394:VAL:HG12	1:A:395:PRO:HD2	1.34	1.06
1:A:142:MET:O	1:A:147:LEU:HB2	1.55	1.05
1:B:32:LEU:HD12	1:B:32:LEU:H	1.18	1.05
1:A:20:MET:CB	1:A:289:LYS:HG3	1.85	1.04
1:B:141:LEU:O	1:B:145:PHE:O	1.78	1.01
2:B:501:HEM:HBB2	2:B:501:HEM:HMB2	1.42	1.01
1:B:15:TYR:HD2	1:B:43:MET:HE2	1.20	1.00
1:B:45:TYR:CD2	1:B:82:PRO:HA	2.00	0.96
1:A:20:MET:CB	1:A:289:LYS:CG	2.44	0.96
1:A:287:ILE:C	1:A:394:VAL:HG13	1.86	0.94
1:A:220:ARG:CD	1:A:225:ARG:HG3	1.97	0.94
1:B:45:TYR:CE2	1:B:82:PRO:CA	2.51	0.93
1:A:220:ARG:HD3	1:A:225:ARG:CG	1.99	0.93
1:B:283:ARG:HG3	1:B:322:ASN:HB3	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:GLU:HG2	1:A:307:ILE:HD12	1.52	0.90
1:B:45:TYR:CE2	1:B:82:PRO:CD	2.54	0.89
1:A:66:ARG:CZ	1:A:301:VAL:HG13	2.03	0.89
1:A:66:ARG:NH1	1:A:301:VAL:HG13	1.87	0.88
1:B:37:GLU:CB	1:B:304:SER:O	2.21	0.88
1:B:45:TYR:CD2	1:B:82:PRO:CA	2.57	0.88
1:B:182:SER:C	1:B:184:GLU:H	1.77	0.87
1:A:142:MET:O	1:A:147:LEU:CB	2.22	0.87
1:A:21:GLU:HB2	1:A:24:GLU:OE1	1.75	0.86
1:A:15:TYR:HH	1:A:29:TYR:HH	0.94	0.86
1:B:279:ASP:OD1	1:B:360:ARG:NH1	2.09	0.85
1:A:268:ARG:NH2	1:A:375:PRO:O	2.09	0.85
1:A:287:ILE:O	1:A:394:VAL:HG11	1.74	0.84
1:A:271:LEU:HB3	1:A:274:ILE:HD11	1.57	0.84
1:A:220:ARG:CD	1:A:225:ARG:CG	2.57	0.83
1:A:15:TYR:C	1:A:17:PHE:HD1	1.81	0.82
1:B:22:ARG:NH1	1:B:384:PRO:HA	1.94	0.82
1:B:45:TYR:CD2	1:B:81:LEU:C	2.53	0.82
1:A:20:MET:CA	1:A:289:LYS:HD2	2.10	0.81
1:B:45:TYR:CE2	1:B:81:LEU:C	2.53	0.80
1:A:271:LEU:O	1:A:274:ILE:HG13	1.81	0.80
1:B:28:GLU:O	1:B:32:LEU:HD12	1.80	0.80
1:A:20:MET:HA	1:A:289:LYS:HD2	1.62	0.80
1:B:15:TYR:CE2	1:B:43:MET:HE3	2.16	0.79
1:B:357:GLN:O	1:B:361:VAL:HG12	1.83	0.79
1:A:15:TYR:N	1:A:16:PRO:CD	2.46	0.79
1:B:45:TYR:HE2	1:B:82:PRO:HD3	1.47	0.78
1:B:86:ASP:OD1	1:B:86:ASP:N	2.16	0.77
1:B:45:TYR:CD2	1:B:82:PRO:N	2.51	0.77
1:B:213:LEU:N	1:B:213:LEU:HD23	2.00	0.77
1:A:394:VAL:CG1	1:A:395:PRO:HD2	2.14	0.76
1:A:357:GLN:O	1:A:361:VAL:HG12	1.86	0.76
1:B:181:TYR:HD1	1:B:181:TYR:H	1.34	0.76
1:A:162:ILE:CD1	1:A:163:GLU:N	2.19	0.75
1:A:268:ARG:CZ	1:A:375:PRO:O	2.35	0.75
1:B:17:PHE:CE2	1:B:28:GLU:OE2	2.40	0.75
2:B:501:HEM:HMC1	2:B:501:HEM:HBC2	1.68	0.75
1:A:377:LEU:HD11	1:A:402:LEU:HD13	1.69	0.73
1:B:15:TYR:CD2	1:B:43:MET:HE2	2.06	0.73
1:A:225:ARG:HG2	1:A:225:ARG:NH2	2.04	0.71
1:A:225:ARG:HG2	1:A:225:ARG:HH21	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:LEU:N	1:A:393:LEU:HD13	2.05	0.71
1:A:20:MET:CB	1:A:289:LYS:CD	2.69	0.71
1:A:15:TYR:O	1:A:17:PHE:N	2.25	0.70
1:B:32:LEU:HD12	1:B:32:LEU:N	2.00	0.69
1:B:45:TYR:CE2	1:B:82:PRO:CB	2.74	0.69
1:A:214:GLY:O	1:A:217:VAL:HG22	1.93	0.69
1:A:218:ARG:O	1:A:218:ARG:HG2	1.92	0.69
1:B:213:LEU:HD23	1:B:213:LEU:H	1.58	0.68
1:B:29:TYR:O	1:B:32:LEU:HD13	1.93	0.68
1:B:45:TYR:CE2	1:B:82:PRO:HD3	2.25	0.67
1:A:217:VAL:HG12	1:A:231:LEU:HD21	1.75	0.67
1:A:38:LEU:HD13	1:A:303:LEU:HD23	1.75	0.67
1:B:369:SER:O	1:B:373:ARG:HB2	1.94	0.67
1:A:265:ALA:O	1:A:269:LYS:CG	2.29	0.66
1:B:32:LEU:CD1	1:B:32:LEU:H	1.96	0.66
1:B:355:GLY:O	1:B:359:VAL:HG23	1.95	0.66
2:B:501:HEM:HBB2	2:B:501:HEM:CMB	2.22	0.65
1:A:109:LEU:O	1:A:109:LEU:HG	1.96	0.65
1:A:36:GLY:O	1:A:37:GLU:C	2.33	0.65
1:A:66:ARG:CZ	1:A:301:VAL:CG1	2.74	0.65
1:B:10:GLY:C	1:B:11:LYS:HG2	2.17	0.65
1:B:52:ALA:HB1	1:B:57:ASP:HB3	1.79	0.65
1:A:38:LEU:HD11	1:A:303:LEU:HD22	1.80	0.64
1:B:149:LEU:O	1:B:149:LEU:HD12	1.97	0.64
1:B:29:TYR:CD2	1:B:317:GLN:HG2	2.33	0.64
1:A:14:PRO:C	1:A:16:PRO:HD2	2.19	0.64
1:A:182:SER:O	1:A:186:VAL:HG13	1.98	0.63
1:A:20:MET:CB	1:A:289:LYS:HD2	2.28	0.63
1:A:309:LYS:O	1:A:312:GLU:HB2	2.00	0.62
1:A:55:TRP:CG	1:A:327:VAL:HG21	2.35	0.62
1:B:45:TYR:HD2	1:B:81:LEU:C	2.01	0.61
1:B:45:TYR:CE2	1:B:82:PRO:HB3	2.35	0.61
1:B:174:GLN:HG2	1:B:181:TYR:CD2	2.35	0.61
2:A:501:HEM:HBC2	2:A:501:HEM:HHD	1.82	0.61
1:B:394:VAL:HB	1:B:395:PRO:HD2	1.83	0.61
1:A:66:ARG:NH2	1:A:301:VAL:HG13	2.16	0.61
1:A:148:PRO:O	1:A:149:LEU:C	2.38	0.61
1:A:120:ARG:O	1:A:124:VAL:HG23	2.01	0.60
1:B:55:TRP:CG	1:B:327:VAL:HG21	2.36	0.60
1:A:14:PRO:HB2	1:A:16:PRO:HD2	1.83	0.60
1:A:287:ILE:C	1:A:394:VAL:CG1	2.57	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:GLN:HE21	1:A:317:GLN:HA	1.67	0.59
1:B:129:ILE:CD1	1:B:374:ILE:HD11	2.32	0.59
1:A:145:PHE:O	1:A:148:PRO:HD2	2.01	0.59
1:A:98:HIS:CE1	1:A:351:HIS:CE1	2.90	0.59
1:B:38:LEU:HD11	1:B:303:LEU:HD23	1.85	0.59
1:B:283:ARG:HB2	1:B:343:HIS:HB2	1.85	0.59
1:A:259:THR:OG1	1:A:383:GLU:OE1	2.21	0.59
1:B:213:LEU:O	1:B:214:GLY:C	2.38	0.59
1:B:10:GLY:O	1:B:11:LYS:HG2	2.01	0.59
1:A:219:ALA:C	1:A:220:ARG:HG2	2.23	0.59
1:B:159:GLY:HA3	1:B:211:ASP:OD2	2.02	0.59
1:A:209:THR:HB	1:A:211:ASP:HB2	1.85	0.58
1:B:195:LEU:O	1:B:199:GLU:CG	2.51	0.58
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.34	0.58
1:A:147:LEU:HB3	1:A:148:PRO:HD3	1.86	0.58
1:A:317:GLN:HA	1:A:317:GLN:NE2	2.19	0.58
1:B:241:ALA:O	3:B:502:E53:C45	2.51	0.58
1:A:283:ARG:NH1	1:A:331:PRO:O	2.37	0.58
1:B:267:LEU:O	1:B:268:ARG:C	2.41	0.58
1:A:390:ARG:CG	1:A:390:ARG:HH21	2.17	0.58
1:A:66:ARG:NH2	1:A:301:VAL:CG1	2.68	0.57
1:B:299:GLU:O	1:B:301:VAL:HG23	2.04	0.57
1:A:38:LEU:CD1	1:A:303:LEU:CD2	2.83	0.57
1:A:258:LEU:HD23	1:A:264:LEU:HD11	1.87	0.57
1:A:220:ARG:CD	1:A:225:ARG:HG2	2.33	0.57
1:B:117:LEU:O	1:B:121:THR:OG1	2.20	0.57
1:A:38:LEU:HD13	1:A:303:LEU:CD2	2.35	0.57
1:A:141:LEU:O	1:A:146:ALA:N	2.36	0.57
1:A:294:VAL:HG22	1:A:313:ALA:HB1	1.87	0.57
1:B:185:VAL:O	1:B:189:ALA:CB	2.53	0.57
1:B:58:VAL:HG12	1:B:316:ILE:HG22	1.87	0.56
1:B:55:TRP:CB	1:B:327:VAL:HG21	2.35	0.56
1:B:146:ALA:O	1:B:150:PRO:CD	2.53	0.56
1:B:182:SER:C	1:B:184:GLU:N	2.42	0.56
1:A:174:GLN:O	1:A:186:VAL:HG12	2.05	0.56
1:A:69:ARG:HD3	1:A:91:MET:O	2.05	0.56
2:A:501:HEM:CBD	2:A:501:HEM:HHA	2.36	0.56
1:B:181:TYR:HD1	1:B:181:TYR:N	2.04	0.55
1:B:181:TYR:N	1:B:181:TYR:CD1	2.73	0.55
1:B:319:HIS:O	1:B:323:THR:OG1	2.24	0.55
1:A:225:ARG:CG	1:A:225:ARG:HH21	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ASP:OD1	1:B:373:ARG:NH2	2.39	0.55
1:A:220:ARG:HH11	1:A:220:ARG:HG3	1.72	0.55
1:A:327:VAL:HG13	1:B:384:PRO:HG2	1.88	0.55
1:B:15:TYR:CD1	1:B:16:PRO:HA	2.42	0.55
1:B:185:VAL:O	1:B:189:ALA:HB2	2.06	0.55
1:B:142:MET:O	1:B:145:PHE:O	2.25	0.55
1:A:15:TYR:O	1:A:17:PHE:CE1	2.56	0.54
1:B:283:ARG:CG	1:B:322:ASN:HB3	2.30	0.54
1:B:381:VAL:HG22	1:B:382:PRO:HD2	1.89	0.54
1:A:183:GLN:HA	1:A:186:VAL:HG22	1.89	0.54
1:B:20:MET:HE1	1:B:395:PRO:HB3	1.90	0.54
1:B:45:TYR:HD2	1:B:81:LEU:O	1.90	0.54
1:A:36:GLY:O	1:A:37:GLU:O	2.25	0.54
1:A:249:ALA:O	1:A:253:SER:HB3	2.07	0.54
1:B:183:GLN:HA	1:B:186:VAL:HG22	1.89	0.54
1:A:38:LEU:CD1	1:A:303:LEU:HD22	2.38	0.53
1:B:159:GLY:O	1:B:204:ARG:NH2	2.42	0.53
1:A:207:GLN:NE2	1:A:209:THR:HG23	2.23	0.53
1:B:25:ILE:HD12	1:B:26:HIS:H	1.73	0.53
1:B:195:LEU:O	1:B:199:GLU:HG2	2.09	0.53
1:B:30:ASN:O	1:B:33:ARG:HB3	2.09	0.53
1:B:367:LEU:O	1:B:369:SER:N	2.42	0.53
1:B:69:ARG:HB3	1:B:92:LEU:HA	1.91	0.53
1:A:28:GLU:HA	1:A:28:GLU:OE1	2.07	0.53
1:A:43:MET:HB3	1:A:79:ARG:O	2.09	0.53
1:B:377:LEU:HD11	1:B:402:LEU:HD13	1.91	0.53
1:A:217:VAL:HG23	1:A:218:ARG:N	2.24	0.52
1:B:204:ARG:O	1:B:207:GLN:O	2.27	0.52
1:B:367:LEU:C	1:B:369:SER:N	2.61	0.52
1:A:393:LEU:HD13	1:A:393:LEU:H	1.74	0.52
1:B:129:ILE:HD11	1:B:374:ILE:HD11	1.92	0.52
1:A:15:TYR:N	1:A:16:PRO:HD2	2.22	0.52
1:A:20:MET:HA	1:A:289:LYS:CD	2.37	0.52
1:A:293:TRP:HA	1:A:293:TRP:CE3	2.44	0.52
1:B:268:ARG:CZ	1:B:375:PRO:O	2.58	0.52
1:A:15:TYR:N	1:A:16:PRO:HD3	2.24	0.52
1:A:109:LEU:CD2	1:A:354:MET:HB2	2.40	0.52
1:A:148:PRO:O	1:A:150:PRO:N	2.42	0.52
1:A:118:ARG:HB3	1:A:119:PRO:HD3	1.92	0.52
1:A:283:ARG:HA	1:A:322:ASN:HD22	1.74	0.52
3:B:502:E53:C45	3:B:502:E53:O13	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:LEU:HD22	2:B:501:HEM:CMB	2.39	0.51
1:A:162:ILE:CD1	1:A:162:ILE:N	2.73	0.51
1:B:45:TYR:HE2	1:B:81:LEU:C	2.02	0.51
1:A:284:ILE:HG23	1:A:285:ILE:HG13	1.93	0.51
1:B:195:LEU:O	1:B:199:GLU:HG3	2.09	0.51
2:A:501:HEM:HHA	2:A:501:HEM:HBD1	1.92	0.51
1:B:367:LEU:C	1:B:369:SER:H	2.13	0.51
1:B:283:ARG:HA	1:B:322:ASN:HD22	1.75	0.51
1:B:341:ASN:OD1	1:B:343:HIS:HB3	2.11	0.51
1:A:145:PHE:CD1	1:A:146:ALA:N	2.79	0.51
1:A:114:MET:HE2	1:A:358:LEU:HB2	1.92	0.51
1:B:29:TYR:O	1:B:32:LEU:CD1	2.58	0.51
1:A:263:LYS:HE2	1:A:334:ILE:O	2.11	0.51
1:A:55:TRP:CB	1:A:327:VAL:HG21	2.41	0.50
1:B:187:MET:O	1:B:191:GLN:N	2.27	0.50
1:B:194:TYR:CD1	1:B:232:VAL:HG11	2.46	0.50
1:A:96:PRO:HD2	1:A:97:GLU:OE2	2.12	0.50
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.93	0.50
1:B:183:GLN:HA	1:B:186:VAL:CG2	2.42	0.50
1:A:15:TYR:C	1:A:17:PHE:CD1	2.69	0.50
1:A:266:GLU:O	1:A:270:ASP:HB3	2.11	0.50
1:A:317:GLN:OE1	1:A:319:HIS:CB	2.60	0.49
1:B:199:GLU:O	1:B:203:GLU:HG2	2.12	0.49
1:A:145:PHE:CD1	1:A:145:PHE:C	2.85	0.49
1:B:66:ARG:NH1	1:B:301:VAL:HG22	2.28	0.49
3:B:502:E53:C33	4:B:603:HOH:O	2.60	0.49
1:B:264:LEU:CD1	1:B:371:ILE:HD11	2.42	0.49
1:A:244:GLU:O	1:A:248:ASN:ND2	2.38	0.49
1:A:372:SER:O	1:A:374:ILE:N	2.44	0.49
1:B:236:VAL:O	1:B:240:ILE:HG13	2.12	0.49
1:B:317:GLN:OE1	1:B:319:HIS:HB3	2.12	0.49
1:A:85:GLN:O	1:A:87:GLN:CD	2.51	0.49
1:A:118:ARG:HH21	1:A:361:VAL:HA	1.76	0.49
1:B:146:ALA:O	1:B:150:PRO:HD3	2.13	0.49
1:B:168:PHE:CE1	1:B:193:LEU:HD11	2.47	0.49
1:A:148:PRO:C	1:A:150:PRO:CD	2.80	0.49
1:A:290:GLN:NE2	1:A:393:LEU:C	2.64	0.49
1:B:389:LEU:HD12	1:B:396:SER:HB2	1.93	0.49
1:A:293:TRP:HA	1:A:293:TRP:HE3	1.78	0.48
1:B:147:LEU:O	1:B:147:LEU:HD23	2.14	0.48
1:A:145:PHE:HD1	1:A:146:ALA:N	2.10	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:GLN:CG	1:B:181:TYR:CD2	2.96	0.48
1:B:282:LEU:O	1:B:283:ARG:C	2.51	0.48
1:B:205:ARG:HG3	1:B:217:VAL:HG11	1.95	0.48
1:B:383:GLU:N	1:B:384:PRO:HD2	2.29	0.48
1:A:390:ARG:CG	1:A:390:ARG:NH2	2.73	0.47
1:B:20:MET:CE	1:B:395:PRO:HB3	2.44	0.47
1:B:69:ARG:O	1:B:72:THR:OG1	2.29	0.47
1:A:147:LEU:N	1:A:148:PRO:HD2	2.29	0.47
1:B:322:ASN:OD1	1:B:343:HIS:O	2.31	0.47
1:A:294:VAL:CG2	1:A:313:ALA:HB1	2.45	0.47
1:A:369:SER:OG	1:A:370:LEU:N	2.48	0.47
1:A:182:SER:OG	1:A:183:GLN:N	2.48	0.47
1:A:292:SER:HB3	1:A:316:ILE:O	2.15	0.47
1:A:87:GLN:N	1:A:88:PRO:CD	2.78	0.47
1:A:207:GLN:HE21	1:A:209:THR:HG23	1.80	0.47
1:A:264:LEU:O	1:A:267:LEU:N	2.48	0.47
1:B:208:ASP:OD1	1:B:218:ARG:HD2	2.15	0.47
1:A:355:GLY:HA3	2:A:501:HEM:C3B	2.50	0.46
1:A:17:PHE:CD1	1:A:17:PHE:N	2.83	0.46
1:A:21:GLU:HB2	1:A:24:GLU:CD	2.34	0.46
1:A:87:GLN:N	1:A:88:PRO:HD3	2.30	0.46
1:B:235:ALA:O	1:B:238:LEU:HB2	2.14	0.46
1:B:31:ARG:O	1:B:34:ASP:N	2.48	0.46
1:B:147:LEU:N	1:B:148:PRO:CD	2.79	0.46
1:A:290:GLN:NE2	1:A:393:LEU:CA	2.79	0.46
1:B:127:ASP:O	1:B:130:ASP:HB2	2.16	0.46
1:A:109:LEU:HD23	1:A:354:MET:HB2	1.97	0.46
1:A:377:LEU:HD11	1:A:402:LEU:CD1	2.42	0.45
1:B:90:ILE:HD13	1:B:101:LEU:HD22	1.98	0.45
1:B:137:ALA:HB1	1:B:403:THR:HA	1.98	0.45
1:A:92:LEU:HD21	1:A:293:TRP:CD1	2.52	0.45
1:A:263:LYS:CE	1:A:334:ILE:O	2.64	0.45
1:A:377:LEU:HD11	1:A:402:LEU:HB3	1.99	0.45
1:A:390:ARG:HA	1:A:390:ARG:HD3	1.51	0.45
1:B:52:ALA:HB2	1:B:303:LEU:HD21	1.97	0.45
1:B:395:PRO:O	1:B:395:PRO:HG2	2.17	0.45
1:B:61:VAL:HG12	1:B:61:VAL:O	2.15	0.45
1:A:282:LEU:O	1:A:283:ARG:C	2.55	0.45
1:B:257:LEU:HG	1:B:281:LEU:HD11	1.99	0.45
1:A:162:ILE:N	1:A:162:ILE:HD12	2.31	0.44
1:A:277:ALA:HA	1:A:336:PHE:CD1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:LEU:HD12	1:A:396:SER:HB2	1.98	0.44
1:A:118:ARG:NH2	1:A:364:GLN:OE1	2.51	0.44
1:A:248:ASN:OD1	1:A:396:SER:HA	2.17	0.44
1:A:376:ALA:O	1:A:378:ARG:CG	2.65	0.44
1:B:45:TYR:CZ	1:B:82:PRO:HB3	2.52	0.44
1:A:142:MET:O	1:A:147:LEU:HB3	2.12	0.44
1:A:147:LEU:N	1:A:148:PRO:CD	2.80	0.44
1:A:217:VAL:CG2	1:A:218:ARG:N	2.81	0.44
1:A:288:ALA:HA	1:A:394:VAL:HA	1.98	0.44
1:B:380:ALA:HB2	1:B:403:THR:HB	1.99	0.44
1:A:288:ALA:HA	1:A:394:VAL:HG13	1.99	0.44
1:A:290:GLN:NE2	1:A:393:LEU:HA	2.33	0.44
1:B:17:PHE:CZ	1:B:28:GLU:OE2	2.71	0.44
1:B:141:LEU:HB3	1:B:400:LEU:HD23	2.00	0.43
1:B:161:PRO:HG2	1:B:164:ASP:OD2	2.17	0.43
1:A:385:ARG:HD3	1:A:385:ARG:HA	1.89	0.43
1:B:129:ILE:HD13	1:B:374:ILE:HD11	1.99	0.43
1:B:264:LEU:HD12	1:B:371:ILE:HD11	2.00	0.43
1:B:189:ALA:O	1:B:193:LEU:HB2	2.18	0.43
1:B:281:LEU:HD23	1:B:281:LEU:HA	1.82	0.43
1:B:26:HIS:CE1	1:B:28:GLU:HB2	2.54	0.43
1:B:149:LEU:HD12	1:B:149:LEU:C	2.38	0.43
1:A:220:ARG:HB3	1:A:224:ASP:O	2.19	0.43
1:A:161:PRO:HG2	1:A:164:ASP:OD2	2.19	0.43
1:B:15:TYR:HB2	1:B:41:VAL:HB	2.01	0.42
1:B:118:ARG:N	1:B:119:PRO:CD	2.82	0.42
1:A:23:LEU:HD13	1:A:285:ILE:HG23	2.01	0.42
1:B:287:ILE:O	1:B:394:VAL:HG12	2.20	0.42
1:A:28:GLU:OE1	1:A:31:ARG:CZ	2.56	0.42
1:A:353:CYS:HA	2:A:501:HEM:C1A	2.55	0.42
1:B:38:LEU:CD1	1:B:303:LEU:HD23	2.49	0.42
1:A:389:LEU:C	1:A:391:GLY:H	2.22	0.42
1:A:92:LEU:HD21	1:A:293:TRP:HD1	1.84	0.42
1:A:268:ARG:NH1	1:A:375:PRO:O	2.53	0.42
1:B:30:ASN:HB3	1:B:33:ARG:NH2	2.35	0.42
1:B:72:THR:CG2	1:B:77:VAL:HG11	2.49	0.42
1:B:141:LEU:O	1:B:145:PHE:C	2.55	0.42
1:A:317:GLN:NE2	1:A:317:GLN:CA	2.83	0.42
1:B:358:LEU:HD23	2:B:501:HEM:HBB1	2.01	0.42
1:A:65:PRO:HG3	1:B:262:GLU:HA	2.01	0.42
1:A:67:PHE:HZ	1:A:303:LEU:CD1	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:GLN:CD	1:A:290:GLN:N	2.73	0.41
1:B:61:VAL:O	1:B:61:VAL:CG1	2.67	0.41
1:A:171:TRP:O	1:A:174:GLN:N	2.52	0.41
1:A:280:GLU:HA	1:A:280:GLU:OE2	2.20	0.41
1:B:120:ARG:O	1:B:124:VAL:HG23	2.20	0.41
1:A:66:ARG:HH12	1:A:301:VAL:HG13	1.76	0.41
1:B:154:ILE:HD13	1:B:154:ILE:HA	1.94	0.41
1:A:220:ARG:NE	1:A:225:ARG:HG2	2.36	0.41
1:B:171:TRP:O	1:B:174:GLN:HB2	2.20	0.41
1:B:355:GLY:O	1:B:359:VAL:CG2	2.66	0.41
1:B:118:ARG:HB3	1:B:119:PRO:HD3	2.03	0.41
1:A:90:ILE:HD12	1:A:101:LEU:HB3	2.03	0.41
1:A:24:GLU:O	1:A:24:GLU:HG2	2.21	0.41
1:A:119:PRO:O	1:A:122:GLN:HB2	2.21	0.41
1:A:381:VAL:HG22	1:A:382:PRO:HD2	2.02	0.41
1:A:105:ALA:HB1	1:A:234:PHE:CZ	2.56	0.41
1:A:199:GLU:O	1:A:202:ALA:HB3	2.20	0.41
1:A:390:ARG:HH21	1:A:390:ARG:HG3	1.84	0.41
1:B:50:TRP:CD1	1:B:308:VAL:HG22	2.56	0.41
1:B:358:LEU:CD2	2:B:501:HEM:HBB1	2.50	0.41
1:B:218:ARG:O	1:B:220:ARG:HD2	2.21	0.41
1:A:14:PRO:C	1:A:16:PRO:CD	2.85	0.40
1:A:355:GLY:HA3	2:A:501:HEM:C2B	2.56	0.40
1:B:44:PRO:HB2	1:B:45:TYR:H	1.75	0.40
1:B:283:ARG:HB2	1:B:343:HIS:CB	2.50	0.40
1:B:383:GLU:O	1:B:386:ILE:HG13	2.21	0.40
1:A:143:GLU:HA	1:A:147:LEU:HD22	2.03	0.40
1:A:167:LYS:O	1:A:167:LYS:HG2	2.21	0.40
1:B:22:ARG:HH21	1:B:22:ARG:CG	2.35	0.40
1:B:174:GLN:CD	1:B:185:VAL:HG11	2.42	0.40
1:A:73:LEU:HD23	1:A:73:LEU:HA	1.91	0.40
1:A:120:ARG:HD2	1:A:120:ARG:HA	1.97	0.40
1:A:318:THR:O	1:A:322:ASN:OD1	2.40	0.40
1:B:45:TYR:N	1:B:45:TYR:CD1	2.87	0.40
1:B:72:THR:HG22	1:B:77:VAL:HG11	2.02	0.40
1:B:105:ALA:HB1	1:B:234:PHE:CZ	2.57	0.40

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	384/404 (95%)	312 (81%)	63 (16%)	9 (2%)	6	30
1	B	389/404 (96%)	330 (85%)	49 (13%)	10 (3%)	5	27
All	All	773/808 (96%)	642 (83%)	112 (14%)	19 (2%)	5	28

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	LEU
1	B	35	ALA
1	B	183	GLN
1	A	35	ALA
1	A	373	ARG
1	B	368	GLY
1	B	21	GLU
1	B	70	SER
1	A	148	PRO
1	A	308	VAL
1	B	222	LYS
1	B	306	THR
1	B	390	ARG
1	A	37	GLU
1	A	264	LEU
1	B	11	LYS
1	A	16	PRO
1	A	294	VAL
1	B	44	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	325/343 (95%)	273 (84%)	52 (16%)	2	12
1	B	325/343 (95%)	283 (87%)	42 (13%)	4	19
All	All	650/686 (95%)	556 (86%)	94 (14%)	3	15

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	PHE
1	A	22	ARG
1	A	23	LEU
1	A	25	ILE
1	A	31	ARG
1	A	40	ARG
1	A	80	VAL
1	A	87	GLN
1	A	91	MET
1	A	97	GLU
1	A	101	LEU
1	A	121	THR
1	A	129	ILE
1	A	135	LYS
1	A	140	ASP
1	A	145	PHE
1	A	151	ILE
1	A	162	ILE
1	A	163	GLU
1	A	173	ASP
1	A	182	SER
1	A	187	MET
1	A	205	ARG
1	A	209	THR
1	A	215	SER
1	A	220	ARG
1	A	225	ARG
1	A	229	THR
1	A	239	LEU
1	A	253	SER
1	A	262	GLU
1	A	268	ARG
1	A	269	LYS

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Mol	Chain	Res	Type
1	A	272	SER
1	A	273	LEU
1	A	283	ARG
1	A	289	LYS
1	A	290	GLN
1	A	292	SER
1	A	299	GLU
1	A	300	ASP
1	A	312	GLU
1	A	316	ILE
1	A	333	GLU
1	A	340	SER
1	A	354	MET
1	A	361	VAL
1	A	369	SER
1	A	378	ARG
1	A	390	ARG
1	A	393	LEU
1	A	394	VAL
1	B	11	LYS
1	B	20	MET
1	B	22	ARG
1	B	23	LEU
1	B	25	ILE
1	B	32	LEU
1	B	38	LEU
1	B	40	ARG
1	B	43	MET
1	B	72	THR
1	B	86	ASP
1	B	102	ARG
1	B	127	ASP
1	B	147	LEU
1	B	154	ILE
1	B	181	TYR
1	B	182	SER
1	B	187	MET
1	B	193	LEU
1	B	204	ARG
1	B	218	ARG
1	B	227	SER
1	B	240	ILE

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Mol	Chain	Res	Type
1	B	246	THR
1	B	252	ASN
1	B	253	SER
1	B	294	VAL
1	B	299	GLU
1	B	318	THR
1	B	323	THR
1	B	335	ASP
1	B	343	HIS
1	B	344	MET
1	B	345	SER
1	B	361	VAL
1	B	369	SER
1	B	371	ILE
1	B	378	ARG
1	B	383	GLU
1	B	385	ARG
1	B	386	ILE
1	B	394	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	207	GLN
1	A	290	GLN
1	B	183	GLN
1	B	348	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 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	#$|Z| > 2$
2	HEM	A	501	1	41,50,50	1.52	9 (21%)	45,82,82	1.71	13 (28%)
2	HEM	B	501	1	41,50,50	1.60	8 (19%)	45,82,82	1.86	13 (28%)
3	E53	B	502	-	68,71,71	1.22	4 (5%)	77,99,99	1.82	20 (25%)

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
2	HEM	A	501	1	-	8/12/54/54	-
2	HEM	B	501	1	-	5/12/54/54	-
3	E53	B	502	-	-	32/85/128/128	0/3/4/4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	E53	O4-C14	5.38	1.46	1.34
3	B	502	E53	C20-C21	-3.97	1.48	1.53
2	B	501	HEM	C4B-NB	-3.42	1.31	1.38
2	A	501	HEM	C4D-ND	-3.41	1.34	1.40
2	B	501	HEM	C3C-C2C	-3.28	1.35	1.40
2	B	501	HEM	C1B-NB	-3.15	1.34	1.40
3	B	502	E53	C11-C13	3.05	1.56	1.53
2	A	501	HEM	C3B-C4B	2.97	1.50	1.44
2	A	501	HEM	FE-NB	2.89	2.11	1.96
2	A	501	HEM	C4B-NB	-2.87	1.32	1.38
2	B	501	HEM	C4D-C3D	2.82	1.49	1.45
2	A	501	HEM	C3C-C2C	-2.81	1.36	1.40
3	B	502	E53	O9-C22	2.78	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	CHB-C1B	2.73	1.42	1.35
2	A	501	HEM	C1B-NB	-2.73	1.35	1.40
2	B	501	HEM	C4D-ND	-2.38	1.36	1.40
2	A	501	HEM	FE-ND	-2.30	1.85	1.96
2	B	501	HEM	FE-NB	2.27	2.08	1.96
2	A	501	HEM	CHB-C1B	2.18	1.40	1.35
2	B	501	HEM	C3B-C4B	2.11	1.49	1.44
2	A	501	HEM	C1D-ND	-2.04	1.34	1.38

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	E53	C51-C50-C49	-5.25	105.83	110.75
3	B	502	E53	C18-C19-N	-5.04	102.76	110.67
3	B	502	E53	C32-C31-C33	-4.58	118.37	124.03
3	B	502	E53	O4-C14-C15	4.48	120.64	110.78
2	B	501	HEM	CAD-C3D-C4D	4.03	131.69	124.66
2	B	501	HEM	CBD-CAD-C3D	3.85	123.33	112.63
2	B	501	HEM	C1B-NB-C4B	3.65	108.84	105.07
2	B	501	HEM	CHD-C1D-ND	3.62	128.36	124.43
2	A	501	HEM	C1B-NB-C4B	3.58	108.77	105.07
2	B	501	HEM	CHC-C4B-NB	3.54	128.27	124.43
2	A	501	HEM	CHD-C1D-ND	3.47	128.20	124.43
3	B	502	E53	O11-C43-C41	-3.42	114.92	121.26
2	B	501	HEM	CHB-C1B-NB	3.33	128.50	124.38
2	A	501	HEM	C4B-CHC-C1C	3.19	126.77	122.56
3	B	502	E53	C17-C16-C15	2.89	116.61	111.23
3	B	502	E53	C6-C5-C4	2.77	118.28	111.71
2	B	501	HEM	CHA-C4D-ND	2.71	127.73	124.38
3	B	502	E53	C53-C52-C50	2.71	121.12	117.72
2	B	501	HEM	O2D-CGD-O1D	-2.63	116.73	123.30
3	B	502	E53	C36-C35-C34	-2.62	118.97	124.81
2	A	501	HEM	O2A-CGA-CBA	2.59	122.34	114.03
2	A	501	HEM	C4B-C3B-C2B	-2.57	105.07	107.11
2	A	501	HEM	CMB-C2B-C1B	2.57	128.95	125.04
3	B	502	E53	C41-C40-C38	2.56	120.50	114.67
3	B	502	E53	C5-C4-C3	2.54	114.29	110.85
2	B	501	HEM	CAD-C3D-C2D	-2.52	123.19	127.88
2	A	501	HEM	CHB-C1B-NB	2.52	127.49	124.38
3	B	502	E53	O4-C14-O5	-2.50	119.27	123.94
2	A	501	HEM	CHA-C4D-ND	2.49	127.46	124.38
3	B	502	E53	O4-C13-C11	2.38	112.21	107.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	HEM	CAD-CBD-CGD	-2.37	108.50	113.60
3	B	502	E53	O13-C46-C44	-2.37	105.85	110.05
3	B	502	E53	C35-C34-C33	-2.37	118.62	123.47
2	A	501	HEM	CHD-C1D-C2D	-2.34	121.33	124.98
3	B	502	E53	C16-C15-N	-2.33	107.28	110.53
2	B	501	HEM	CMA-C3A-C4A	-2.33	124.89	128.46
2	A	501	HEM	C4D-ND-C1D	2.32	107.47	105.07
2	A	501	HEM	CHC-C4B-NB	2.29	126.92	124.43
2	A	501	HEM	CAD-C3D-C4D	2.28	128.64	124.66
3	B	502	E53	C28-C23-C24	-2.17	108.82	113.83
2	A	501	HEM	CAB-C3B-C2B	-2.12	121.62	128.60
3	B	502	E53	C24-C25-C26	-2.08	109.33	112.65
3	B	502	E53	C28-C29-C31	-2.07	110.61	113.50
3	B	502	E53	O8-C23-C24	2.06	112.70	110.10
2	B	501	HEM	CHD-C1D-C2D	-2.01	121.83	124.98
2	B	501	HEM	O2D-CGD-CBD	2.01	120.48	114.03

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	HEM	C2D-C3D-CAD-CBD
3	B	502	E53	C11-C10-C6-C5
3	B	502	E53	C11-C10-C6-C7
3	B	502	E53	C47-C49-C50-C52
3	B	502	E53	O13-C46-C47-C49
3	B	502	E53	C44-C46-C47-C49
3	B	502	E53	O13-C46-C47-C48
3	B	502	E53	C44-C46-C47-C48
3	B	502	E53	O12-C44-C46-C47
3	B	502	E53	C43-C44-C46-C47
3	B	502	E53	O12-C44-C46-O13
3	B	502	E53	C43-C44-C46-O13
3	B	502	E53	C43-C44-O12-C45
3	B	502	E53	O11-C43-C44-O12
3	B	502	E53	C41-C43-C44-O12
3	B	502	E53	C39-C38-C40-C41
3	B	502	E53	C37-C38-C40-C41
3	B	502	E53	C23-C28-C29-C31
3	B	502	E53	C23-C28-C29-O10
3	B	502	E53	C21-C20-N-C15
3	B	502	E53	C21-C20-N-C19

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Mol	Chain	Res	Type	Atoms
3	B	502	E53	O6-C20-N-C15
3	B	502	E53	O6-C20-N-C19
3	B	502	E53	C15-C14-O4-C13
2	A	501	HEM	C4D-C3D-CAD-CBD
3	B	502	E53	O5-C14-O4-C13
3	B	502	E53	O5-C14-C15-N
3	B	502	E53	O4-C14-C15-N
2	B	501	HEM	C4D-C3D-CAD-CBD
2	B	501	HEM	C2D-C3D-CAD-CBD
3	B	502	E53	C46-C44-O12-C45
3	B	502	E53	C47-C49-C50-C51
3	B	502	E53	C41-C43-C44-C46
2	A	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C2A-CAA-CBA-CGA
3	B	502	E53	C40-C41-C43-C44
3	B	502	E53	C40-C41-C43-O11
2	A	501	HEM	CAD-CBD-CGD-O1D
2	A	501	HEM	CAD-CBD-CGD-O2D
2	B	501	HEM	CAA-CBA-CGA-O2A
2	B	501	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	C3D-CAD-CBD-CGD
3	B	502	E53	C1-C2-O2-C3

There are no ring outliers.

3 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	7	0
2	B	501	HEM	7	0
3	B	502	E53	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 HEM A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand E53 B 502

Bond lengths

Bond angles

Torsions

Rings
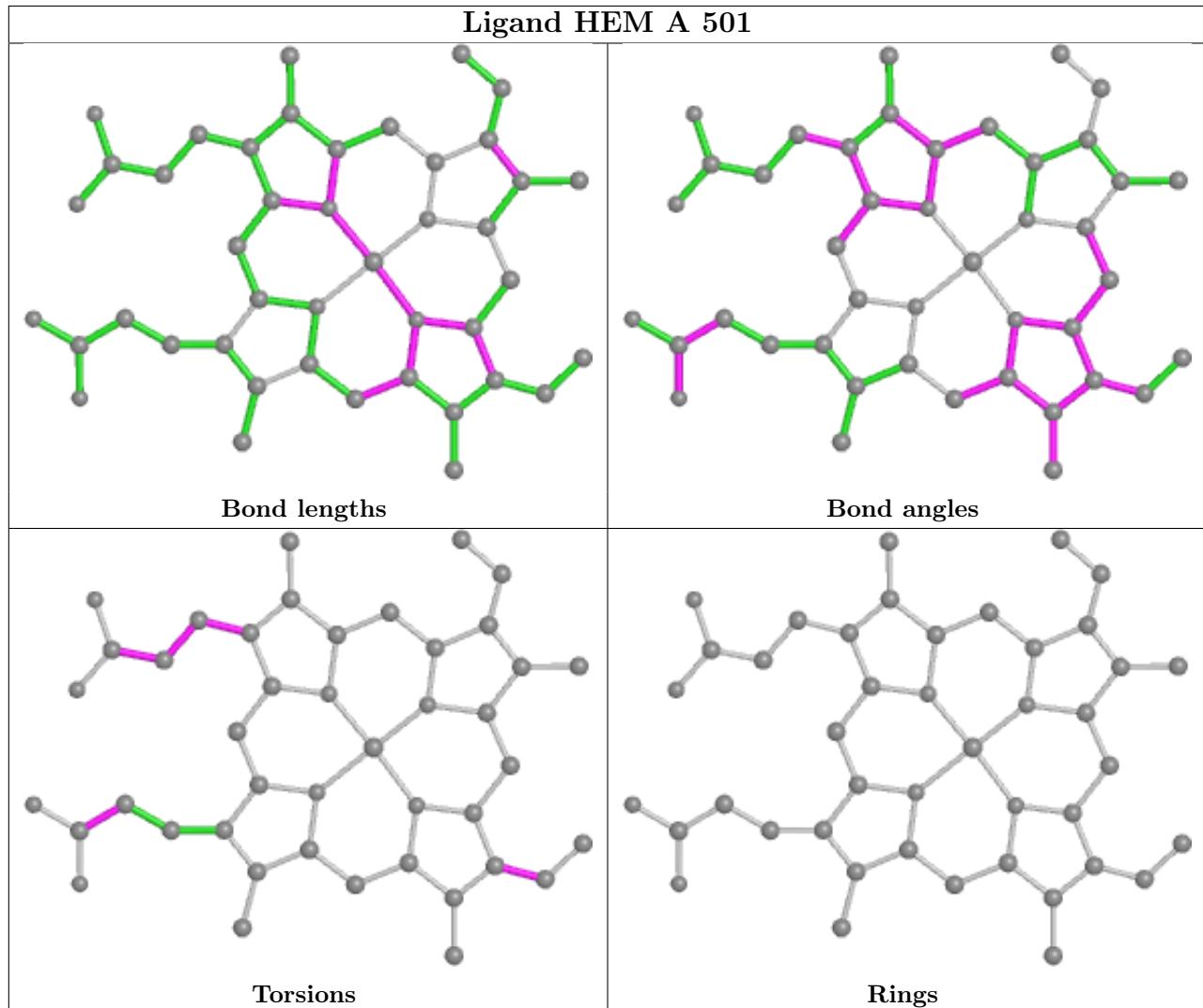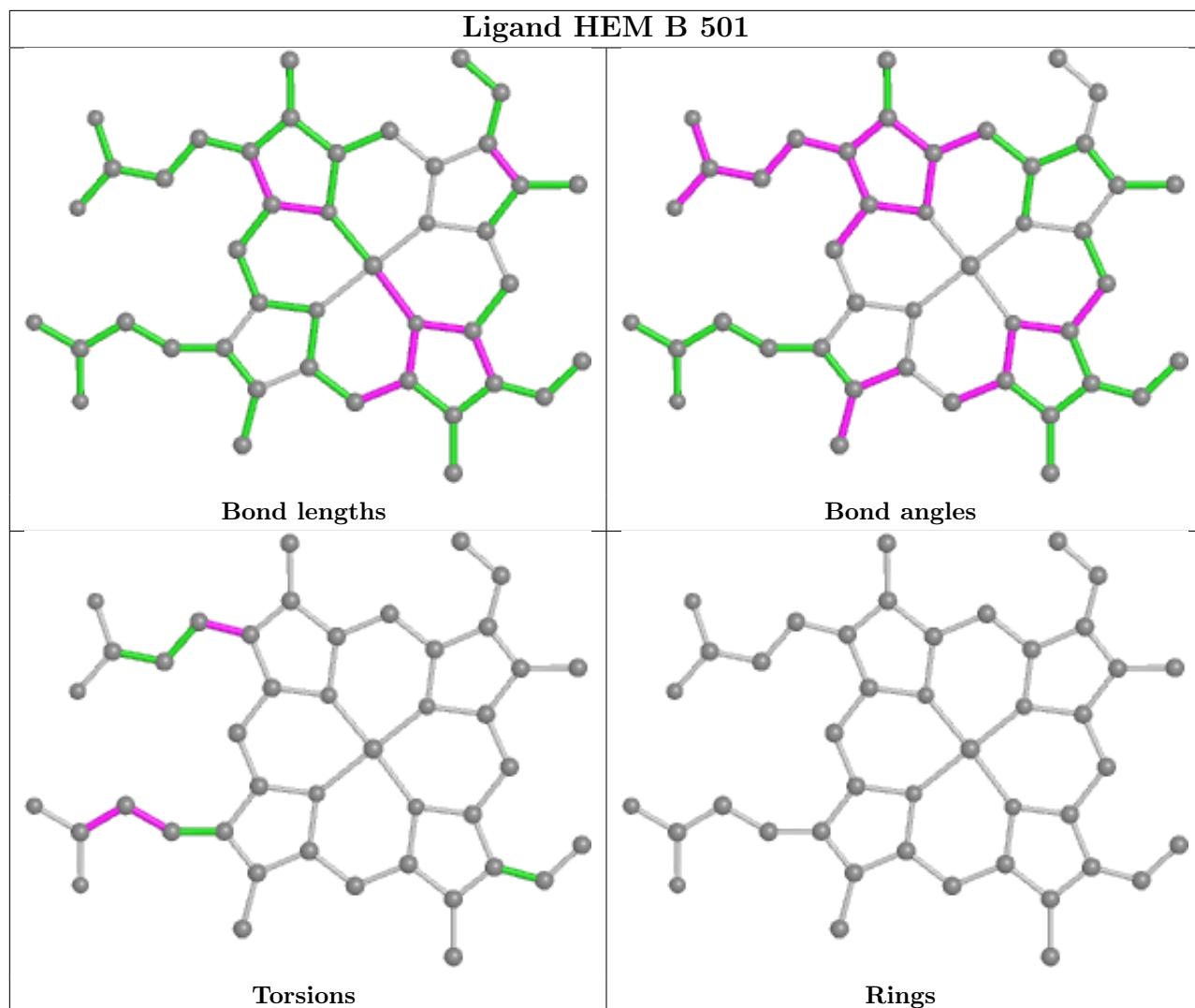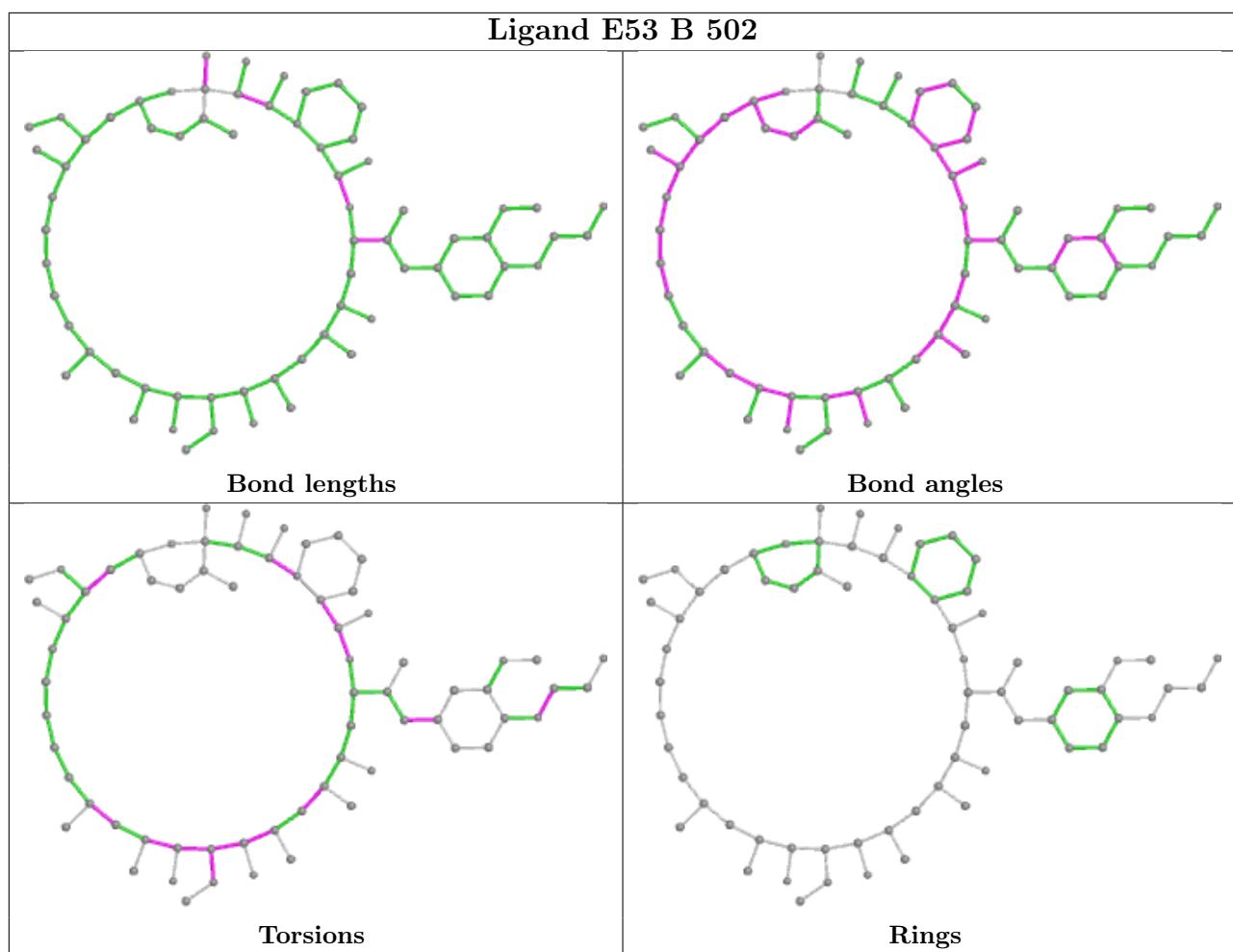
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	390/404 (96%)	-0.10	1 (0%) 94	84	47, 75, 109, 131	0
1	B	393/404 (97%)	-0.08	3 (0%) 86	65	44, 78, 112, 147	0
All	All	783/808 (96%)	-0.09	4 (0%) 91	75	44, 77, 111, 147	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	37	GLU	3.3
1	B	315	ALA	2.2
1	B	83	ALA	2.2
1	A	315	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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(Å²)	Q<0.9
3	E53	B	502	68/68	0.71	0.53	83,138,185,218	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	A	501	43/43	0.95	0.36	51,62,78,88	0
2	HEM	B	501	43/43	0.96	0.34	50,63,79,83	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 E53 B 502:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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 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)
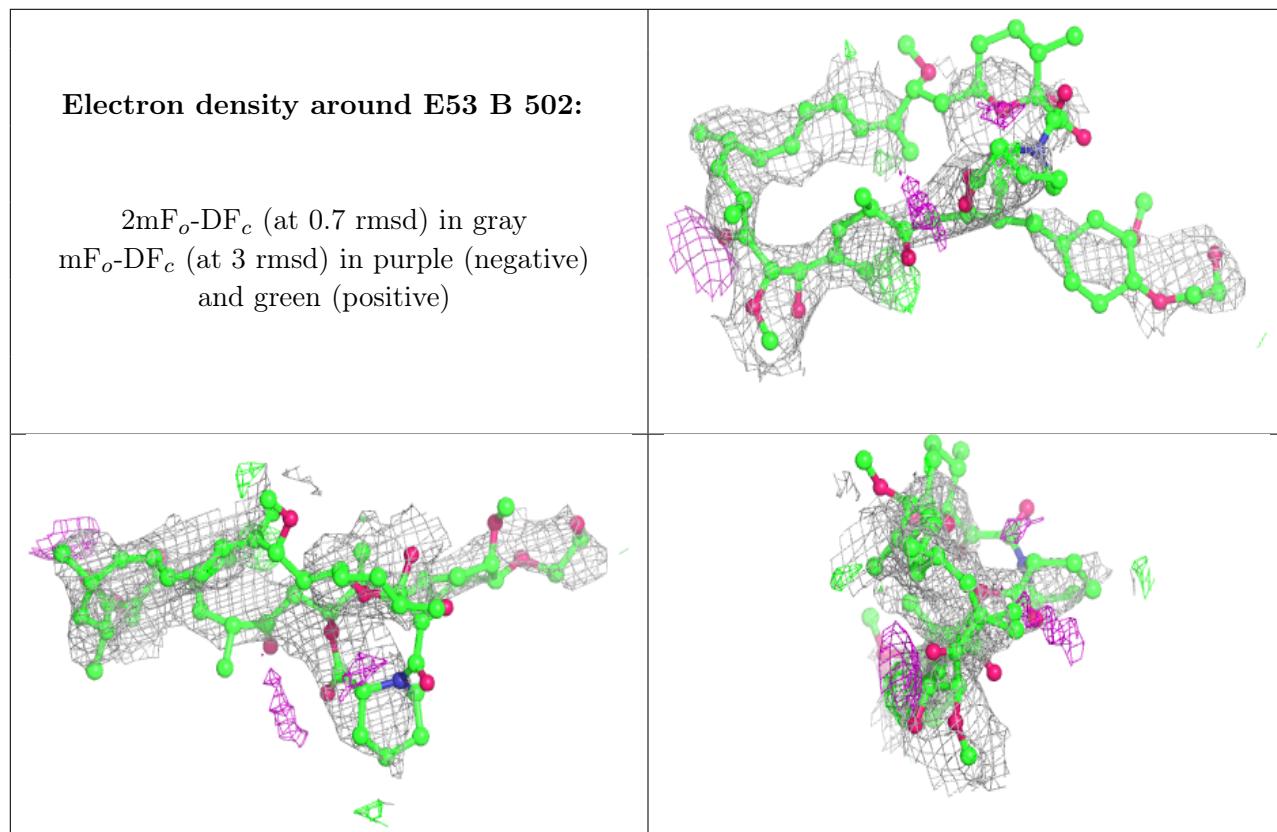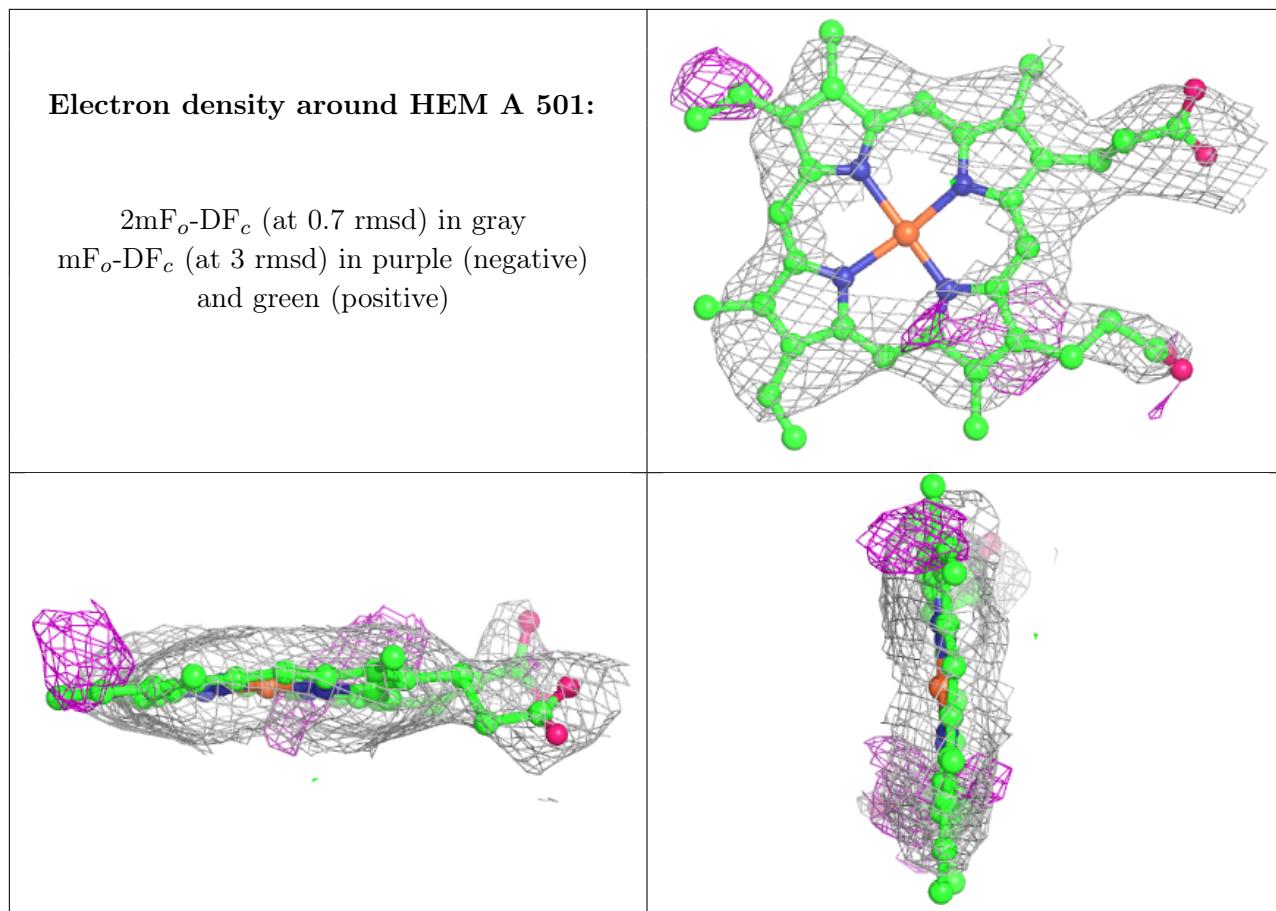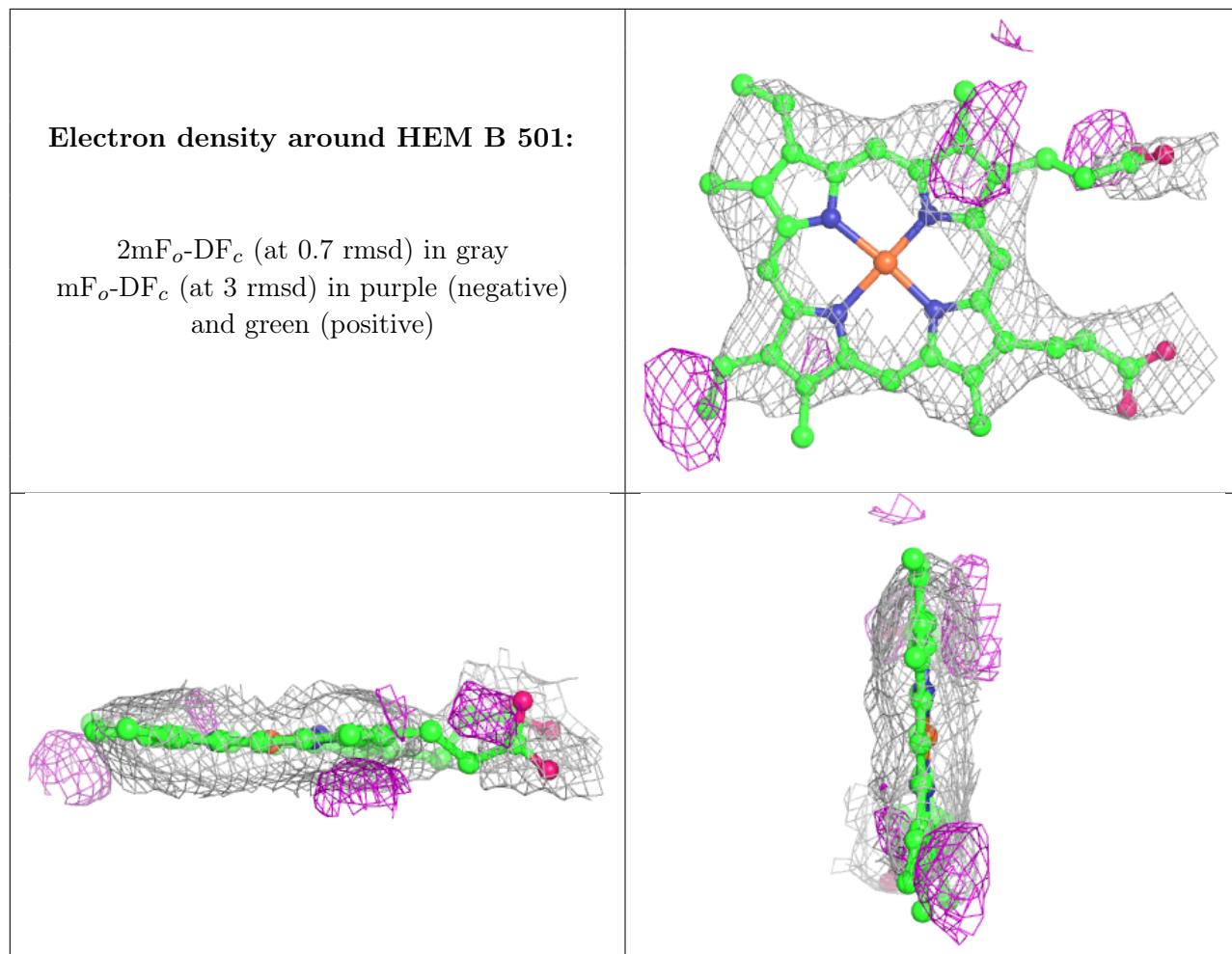
6.5 Other polymers (i)

There are no such residues in this entry.