



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 16, 2026 – 08:08 AM JST

PDB ID : 9L7R / pdb_0000917r
Title : Crystal structure of P450cam-F87R mutant complex with (-)-ambroxide
Authors : Dong, S.; Feng, Y.G.
Deposited on : 2024-12-27
Resolution : 2.04 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 : 1.8.5 (274361), CSD as541be (2020)
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

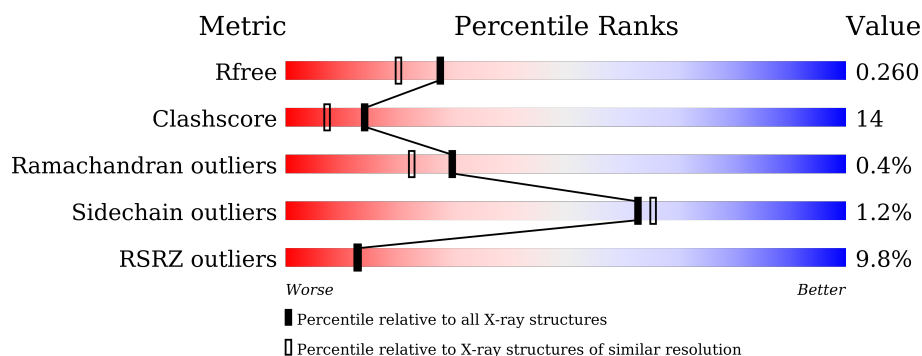
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	467	4% 67%18%14%
1	B	467	13% 66%19%14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6702 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 Camphor 5-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	0	0
			3167	2005	556	589	17			
1	B	400	Total	C	N	O	S	0	0	0
			3151	1994	553	587	17			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-52	MET	-	initiating methionine	UNP P00183
A	-51	HIS	-	expression tag	UNP P00183
A	-50	HIS	-	expression tag	UNP P00183
A	-49	HIS	-	expression tag	UNP P00183
A	-48	HIS	-	expression tag	UNP P00183
A	-47	HIS	-	expression tag	UNP P00183
A	-46	HIS	-	expression tag	UNP P00183
A	-45	SER	-	expression tag	UNP P00183
A	-44	SER	-	expression tag	UNP P00183
A	-43	GLY	-	expression tag	UNP P00183
A	-42	LEU	-	expression tag	UNP P00183
A	-41	VAL	-	expression tag	UNP P00183
A	-40	PRO	-	expression tag	UNP P00183
A	-39	ARG	-	expression tag	UNP P00183
A	-38	GLY	-	expression tag	UNP P00183
A	-37	SER	-	expression tag	UNP P00183
A	-36	GLY	-	expression tag	UNP P00183
A	-35	MET	-	expression tag	UNP P00183
A	-34	LYS	-	expression tag	UNP P00183
A	-33	GLU	-	expression tag	UNP P00183
A	-32	THR	-	expression tag	UNP P00183
A	-31	ALA	-	expression tag	UNP P00183
A	-30	ALA	-	expression tag	UNP P00183
A	-29	ALA	-	expression tag	UNP P00183
A	-28	LYS	-	expression tag	UNP P00183

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	PHE	-	expression tag	UNP P00183
A	-26	GLU	-	expression tag	UNP P00183
A	-25	ARG	-	expression tag	UNP P00183
A	-24	GLN	-	expression tag	UNP P00183
A	-23	HIS	-	expression tag	UNP P00183
A	-22	MET	-	expression tag	UNP P00183
A	-21	ASP	-	expression tag	UNP P00183
A	-20	SER	-	expression tag	UNP P00183
A	-19	PRO	-	expression tag	UNP P00183
A	-18	ASP	-	expression tag	UNP P00183
A	-17	LEU	-	expression tag	UNP P00183
A	-16	GLY	-	expression tag	UNP P00183
A	-15	THR	-	expression tag	UNP P00183
A	-14	ASP	-	expression tag	UNP P00183
A	-13	ASP	-	expression tag	UNP P00183
A	-12	ASP	-	expression tag	UNP P00183
A	-11	ASP	-	expression tag	UNP P00183
A	-10	LYS	-	expression tag	UNP P00183
A	-9	ALA	-	expression tag	UNP P00183
A	-8	MET	-	expression tag	UNP P00183
A	-7	ALA	-	expression tag	UNP P00183
A	-6	ASP	-	expression tag	UNP P00183
A	-5	ILE	-	expression tag	UNP P00183
A	-4	GLY	-	expression tag	UNP P00183
A	-3	SER	-	expression tag	UNP P00183
A	-2	GLU	-	expression tag	UNP P00183
A	-1	PHE	-	expression tag	UNP P00183
A	87	ARG	PHE	engineered mutation	UNP P00183
A	334	ALA	CYS	conflict	UNP P00183
B	-52	MET	-	initiating methionine	UNP P00183
B	-51	HIS	-	expression tag	UNP P00183
B	-50	HIS	-	expression tag	UNP P00183
B	-49	HIS	-	expression tag	UNP P00183
B	-48	HIS	-	expression tag	UNP P00183
B	-47	HIS	-	expression tag	UNP P00183
B	-46	HIS	-	expression tag	UNP P00183
B	-45	SER	-	expression tag	UNP P00183
B	-44	SER	-	expression tag	UNP P00183
B	-43	GLY	-	expression tag	UNP P00183
B	-42	LEU	-	expression tag	UNP P00183
B	-41	VAL	-	expression tag	UNP P00183
B	-40	PRO	-	expression tag	UNP P00183

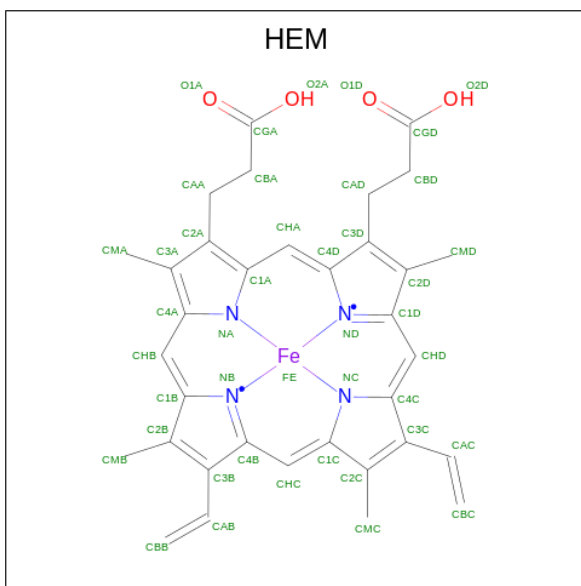
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-39	ARG	-	expression tag	UNP P00183
B	-38	GLY	-	expression tag	UNP P00183
B	-37	SER	-	expression tag	UNP P00183
B	-36	GLY	-	expression tag	UNP P00183
B	-35	MET	-	expression tag	UNP P00183
B	-34	LYS	-	expression tag	UNP P00183
B	-33	GLU	-	expression tag	UNP P00183
B	-32	THR	-	expression tag	UNP P00183
B	-31	ALA	-	expression tag	UNP P00183
B	-30	ALA	-	expression tag	UNP P00183
B	-29	ALA	-	expression tag	UNP P00183
B	-28	LYS	-	expression tag	UNP P00183
B	-27	PHE	-	expression tag	UNP P00183
B	-26	GLU	-	expression tag	UNP P00183
B	-25	ARG	-	expression tag	UNP P00183
B	-24	GLN	-	expression tag	UNP P00183
B	-23	HIS	-	expression tag	UNP P00183
B	-22	MET	-	expression tag	UNP P00183
B	-21	ASP	-	expression tag	UNP P00183
B	-20	SER	-	expression tag	UNP P00183
B	-19	PRO	-	expression tag	UNP P00183
B	-18	ASP	-	expression tag	UNP P00183
B	-17	LEU	-	expression tag	UNP P00183
B	-16	GLY	-	expression tag	UNP P00183
B	-15	THR	-	expression tag	UNP P00183
B	-14	ASP	-	expression tag	UNP P00183
B	-13	ASP	-	expression tag	UNP P00183
B	-12	ASP	-	expression tag	UNP P00183
B	-11	ASP	-	expression tag	UNP P00183
B	-10	LYS	-	expression tag	UNP P00183
B	-9	ALA	-	expression tag	UNP P00183
B	-8	MET	-	expression tag	UNP P00183
B	-7	ALA	-	expression tag	UNP P00183
B	-6	ASP	-	expression tag	UNP P00183
B	-5	ILE	-	expression tag	UNP P00183
B	-4	GLY	-	expression tag	UNP P00183
B	-3	SER	-	expression tag	UNP P00183
B	-2	GLU	-	expression tag	UNP P00183
B	-1	PHE	-	expression tag	UNP P00183
B	87	ARG	PHE	engineered mutation	UNP P00183
B	334	ALA	CYS	conflict	UNP P00183

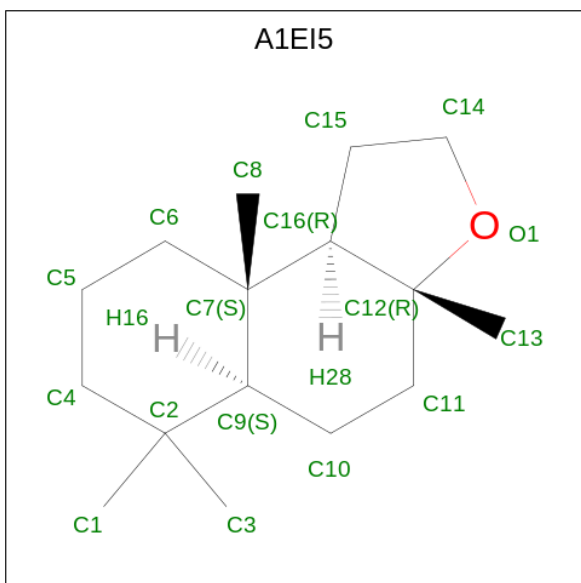
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:

C₃₄H₃₂FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 (3 {a} {R},5 {a} {S},9 {a} {S},9 {b} {R})-3 {a},6,6,9 {a}-tetramethyl-2,4,5,5 {a},7,8,9,9 {b}-octahydro-1 {H}-benzo[e][1]benzofuran (CCD ID: A1EI5) (formula: C₁₆H₂₈O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			17	16	1		
3	B	1	Total	C	O	0	0
			17	16	1		

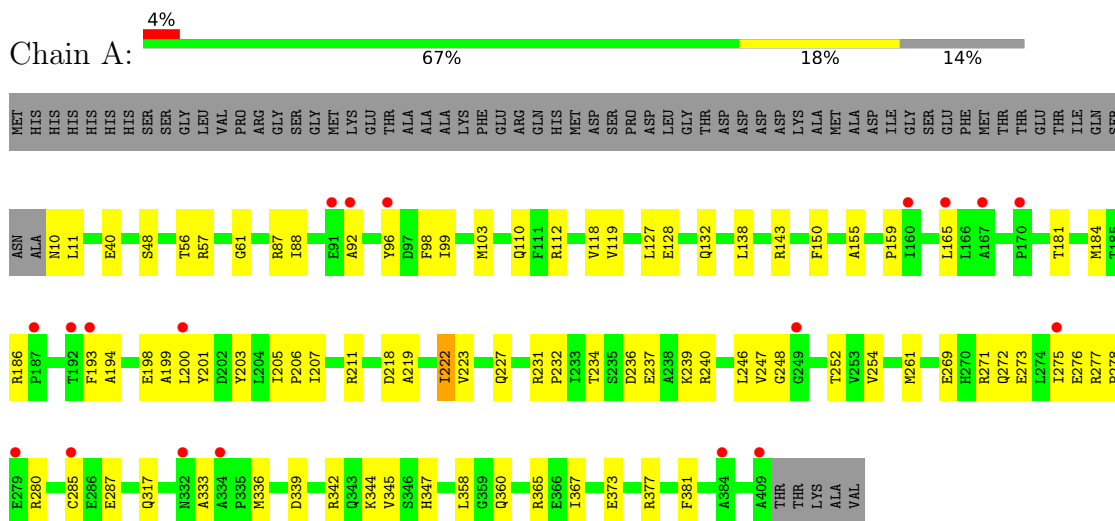
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	125	Total	O	0	0
			125	125		
4	B	139	Total	O	0	0
			139	139		

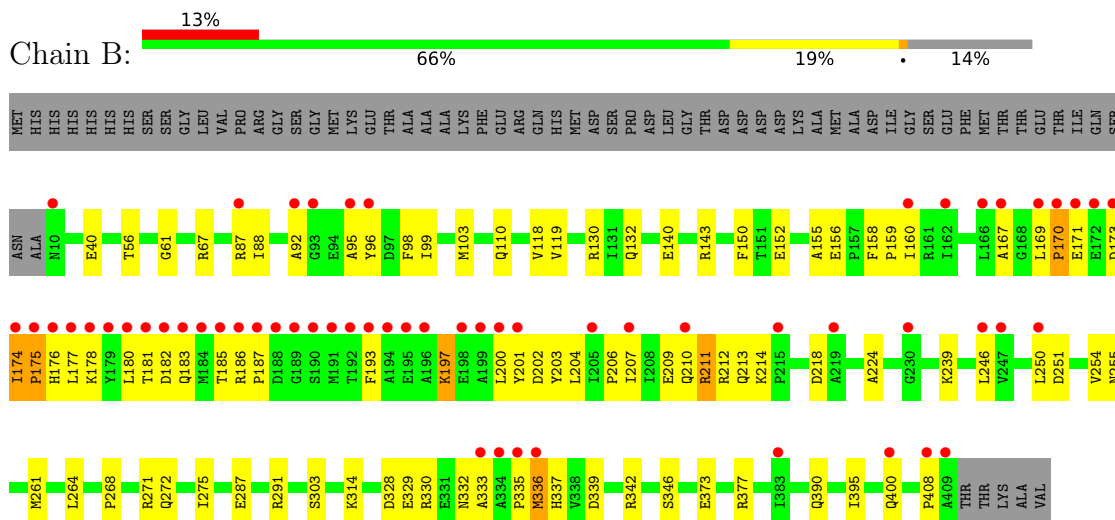
3 Residue-property plots

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: Camphor 5-monooxygenase



• Molecule 1: Camphor 5-monooxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	36.49Å 62.07Å 96.13Å 79.24° 80.85° 75.42°	Depositor
Resolution (Å)	29.82 – 2.04 29.82 – 2.04	Depositor EDS
% Data completeness (in resolution range)	92.7 (29.82-2.04) 88.4 (29.82-2.04)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.03Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.211 , 0.255 0.225 , 0.260	Depositor DCC
R_{free} test set	2008 reflections (4.26%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.041 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6702	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.09 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3879e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, A1EI5

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	0.25	0/3245	0.40	0/4410
1	B	0.21	0/3227	0.42	0/4386
All	All	0.23	0/6472	0.41	0/8796

There are no bond length outliers.

There are no bond angle outliers.

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	3167	0	3108	79	0
1	B	3151	0	3088	99	0
2	A	43	0	30	2	0
2	B	43	0	30	2	0
3	A	17	0	0	0	0
3	B	17	0	0	0	0
4	A	125	0	0	5	1
4	B	139	0	0	6	2
All	All	6702	0	6256	181	3

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 14.

All (181) 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:333:ALA:O	1:B:342:ARG:NH1	1.74	1.17
1:B:87:ARG:HE	1:B:395:ILE:HD11	1.24	1.03
1:B:160:ILE:HD13	1:B:174:ILE:HG21	1.44	1.00
1:B:169:LEU:HB3	1:B:170:PRO:HD2	1.44	0.98
1:B:176:HIS:O	1:B:180:LEU:HD13	1.64	0.96
1:B:177:LEU:HD21	1:B:246:LEU:HD21	1.47	0.95
1:A:99:ILE:HG12	1:A:103:MET:HE3	1.55	0.89
1:B:174:ILE:HB	1:B:178:LYS:HG2	1.58	0.86
1:A:205:ILE:HG13	1:A:206:PRO:HD3	1.56	0.85
1:B:180:LEU:CD2	1:B:200:LEU:HD23	2.07	0.84
1:B:87:ARG:HD3	1:B:92:ALA:HB1	1.60	0.83
1:B:180:LEU:HD23	1:B:200:LEU:HD23	1.58	0.83
1:B:185:THR:HG21	1:B:251:ASP:OD2	1.79	0.82
1:B:160:ILE:HD13	1:B:174:ILE:CG2	2.12	0.80
1:B:132:GLN:NE2	4:B:602:HOH:O	2.14	0.80
1:B:87:ARG:HE	1:B:395:ILE:CD1	1.97	0.78
1:B:169:LEU:HB3	1:B:170:PRO:CD	2.14	0.77
1:B:211:ARG:HG2	1:B:211:ARG:HH21	1.50	0.77
1:A:87:ARG:HD3	1:A:92:ALA:HB1	1.67	0.76
1:B:183:GLN:O	1:B:187:PRO:HD3	1.85	0.76
1:A:333:ALA:O	1:A:342:ARG:NH1	2.20	0.74
1:B:177:LEU:HD21	1:B:246:LEU:CD2	2.17	0.71
1:A:285:CYS:SG	1:A:367:ILE:HG21	2.31	0.70
1:A:277:ARG:HH21	1:A:280:ARG:HD2	1.57	0.70
1:B:174:ILE:N	1:B:175:PRO:HD3	2.06	0.70
1:B:251:ASP:O	1:B:255:ASN:ND2	2.25	0.69
1:A:285:CYS:SG	1:A:367:ILE:CG2	2.80	0.69
1:A:373:GLU:O	1:A:377:ARG:HD2	1.93	0.69
1:B:332:ASN:OD1	4:B:601:HOH:O	2.12	0.67
1:A:118:VAL:HG23	1:A:119:VAL:HG13	1.77	0.66
1:B:390:GLN:HB3	1:B:400:GLN:OE1	1.94	0.66
1:A:277:ARG:NE	1:A:280:ARG:HE	1.94	0.65
1:A:194:ALA:O	1:A:198:GLU:HG3	1.96	0.65
1:A:205:ILE:HG13	1:A:206:PRO:CD	2.26	0.65
1:A:231:ARG:NH2	1:A:234:THR:HG23	2.11	0.64
1:A:99:ILE:HD12	1:A:240:ARG:HB2	1.80	0.64
1:A:339:ASP:O	1:A:342:ARG:HG3	1.98	0.64
1:B:332:ASN:HD21	1:B:346:SER:HB3	1.63	0.64
1:A:218:ASP:O	1:A:222:ILE:HG22	1.99	0.62
1:B:211:ARG:HH21	1:B:211:ARG:CG	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ARG:NH1	1:A:218:ASP:OD2	2.32	0.62
1:B:180:LEU:CD2	1:B:200:LEU:CD2	2.78	0.61
1:B:180:LEU:HD23	1:B:200:LEU:HB2	1.82	0.61
1:A:87:ARG:HH11	1:A:92:ALA:HB1	1.64	0.61
1:B:174:ILE:O	1:B:178:LYS:HG2	2.00	0.61
1:B:176:HIS:O	1:B:180:LEU:CD1	2.43	0.61
1:A:231:ARG:HH22	1:A:234:THR:HG23	1.63	0.61
1:A:150:PHE:CE2	1:A:155:ALA:HB2	2.35	0.61
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.81	0.61
1:A:277:ARG:HH21	1:A:280:ARG:CD	2.13	0.60
1:B:87:ARG:HH11	1:B:92:ALA:HB1	1.66	0.60
1:B:212:ARG:HG3	1:B:224:ALA:HB1	1.82	0.60
1:B:180:LEU:HD22	1:B:200:LEU:HD23	1.84	0.60
1:A:96:TYR:CZ	1:A:98:PHE:HB2	2.37	0.60
1:A:277:ARG:HE	1:A:280:ARG:HE	1.47	0.60
1:B:118:VAL:HG23	1:B:119:VAL:HG13	1.84	0.60
1:A:277:ARG:NE	1:A:280:ARG:NE	2.50	0.60
1:B:183:GLN:HA	1:B:187:PRO:HA	1.83	0.60
1:B:87:ARG:HD3	1:B:92:ALA:CB	2.31	0.59
1:B:110:GLN:NE2	4:B:610:HOH:O	2.35	0.59
1:A:231:ARG:NH1	1:A:237:GLU:OE2	2.22	0.59
1:A:344:LYS:HG2	4:A:613:HOH:O	2.03	0.59
1:B:239:LYS:NZ	4:B:607:HOH:O	2.31	0.59
1:B:209:GLU:OE2	1:B:213:GLN:NE2	2.36	0.58
1:B:140:GLU:HG2	1:B:377:ARG:HH11	1.69	0.58
1:B:87:ARG:NE	1:B:395:ILE:HD11	2.07	0.58
1:B:180:LEU:HD23	1:B:200:LEU:CD2	2.31	0.58
1:B:268:PRO:O	1:B:272:GLN:HG2	2.02	0.58
1:B:143:ARG:NH1	1:B:408:PRO:O	2.30	0.58
1:A:40:GLU:HG3	1:A:336:MET:HE2	1.86	0.58
1:A:10:ASN:N	4:A:610:HOH:O	2.37	0.57
1:A:110:GLN:H	1:A:110:GLN:CD	2.12	0.57
1:A:344:LYS:O	1:A:344:LYS:HG3	2.05	0.57
1:A:269:GLU:CD	1:A:269:GLU:H	2.13	0.56
1:A:287:GLU:CD	1:A:342:ARG:HD2	2.31	0.56
1:B:329:GLU:OE2	1:B:329:GLU:N	2.23	0.56
1:A:287:GLU:OE1	1:A:342:ARG:HD2	2.06	0.56
1:B:143:ARG:HH12	1:B:408:PRO:C	2.12	0.56
1:A:236:ASP:OD1	1:A:239:LYS:NZ	2.35	0.56
1:A:143:ARG:HH11	1:A:143:ARG:HG2	1.72	0.54
1:A:277:ARG:HH21	1:A:280:ARG:NE	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:VAL:HG11	1:A:223:VAL:HG23	1.90	0.54
1:A:128:GLU:HG3	1:A:365:ARG:HD2	1.88	0.54
1:A:199:ALA:O	4:A:602:HOH:O	2.18	0.54
1:B:332:ASN:ND2	1:B:346:SER:HB3	2.23	0.53
1:B:160:ILE:CD1	1:B:174:ILE:HG21	2.29	0.53
2:B:501:HEM:HMB2	2:B:501:HEM:HBB2	1.91	0.53
1:B:328:ASP:OD1	1:B:330:ARG:HG3	2.09	0.53
1:A:219:ALA:O	1:A:222:ILE:HG23	2.09	0.52
1:A:200:LEU:HD21	1:A:246:LEU:HD13	1.92	0.52
1:B:174:ILE:N	1:B:175:PRO:CD	2.73	0.52
1:A:277:ARG:HE	1:A:280:ARG:NE	2.09	0.51
1:A:203:TYR:O	1:A:207:ILE:HD13	2.10	0.51
1:B:177:LEU:HD11	1:B:246:LEU:HD11	1.91	0.51
1:A:201:TYR:O	1:A:205:ILE:HG23	2.09	0.51
1:B:160:ILE:HG12	1:B:250:LEU:HD13	1.92	0.50
1:B:329:GLU:H	1:B:329:GLU:CD	2.13	0.50
1:B:40:GLU:HG3	1:B:336:MET:HE2	1.93	0.50
1:B:67:ARG:NH2	4:B:608:HOH:O	2.44	0.50
1:B:373:GLU:OE2	4:B:602:HOH:O	2.19	0.50
1:A:272:GLN:O	1:A:276:GLU:HG2	2.12	0.50
1:A:277:ARG:NH2	1:A:280:ARG:NE	2.59	0.50
1:A:201:TYR:CD2	1:A:239:LYS:HE2	2.47	0.50
1:B:211:ARG:CG	1:B:211:ARG:NH2	2.73	0.50
1:B:183:GLN:O	1:B:187:PRO:CD	2.57	0.49
1:B:339:ASP:O	1:B:342:ARG:HG3	2.13	0.49
1:A:48:SER:O	1:B:130:ARG:NH1	2.43	0.49
1:A:248:GLY:O	1:A:252:THR:OG1	2.29	0.49
1:B:87:ARG:HG2	1:B:88:ILE:N	2.28	0.49
1:B:202:ASP:O	1:B:206:PRO:HD3	2.12	0.48
1:A:150:PHE:CZ	1:A:261:MET:HG3	2.49	0.48
1:A:231:ARG:NH2	1:A:237:GLU:OE1	2.41	0.48
1:A:143:ARG:HG2	1:A:143:ARG:NH1	2.29	0.48
1:A:205:ILE:HG22	1:A:239:LYS:HD2	1.96	0.48
1:B:246:LEU:O	1:B:250:LEU:HG	2.14	0.48
1:B:206:PRO:O	1:B:210:GLN:HG2	2.13	0.48
1:B:390:GLN:HB3	1:B:400:GLN:CD	2.39	0.48
1:B:390:GLN:CG	1:B:400:GLN:CD	2.86	0.48
1:A:11:LEU:HD22	1:A:57:ARG:HB2	1.96	0.47
1:A:88:ILE:HD11	1:A:317:GLN:HB3	1.97	0.47
1:B:96:TYR:CE1	1:B:98:PHE:HB2	2.49	0.47
1:A:276:GLU:O	1:A:278:PRO:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:VAL:CG1	1:A:222:ILE:HG12	2.45	0.47
1:B:87:ARG:HH11	1:B:92:ALA:CB	2.28	0.47
1:A:181:THR:HG22	1:A:247:VAL:HG22	1.96	0.46
1:B:99:ILE:HG12	1:B:103:MET:HE3	1.98	0.46
1:B:180:LEU:HD23	1:B:200:LEU:CB	2.45	0.46
1:A:127:LEU:HD23	1:A:127:LEU:HA	1.71	0.46
1:B:197:LYS:HE3	1:B:201:TYR:HE2	1.80	0.46
1:A:227:GLN:HB3	1:A:232:PRO:HA	1.98	0.46
1:A:285:CYS:SG	1:A:367:ILE:HG22	2.56	0.45
1:A:112:ARG:HG3	1:A:358:LEU:HD11	1.98	0.45
2:A:501:HEM:HBB2	2:A:501:HEM:HMB2	1.98	0.45
1:B:390:GLN:CB	1:B:400:GLN:OE1	2.64	0.45
1:A:150:PHE:CE1	1:A:261:MET:HG3	2.51	0.45
1:B:95:ALA:HB3	1:B:193:PHE:HD2	1.81	0.45
1:B:96:TYR:CZ	1:B:98:PHE:HB2	2.52	0.45
1:A:181:THR:HA	1:A:184:MET:HE2	1.99	0.45
1:B:150:PHE:CZ	1:B:261:MET:HG3	2.50	0.45
1:B:303:SER:HA	1:B:314:LYS:HB2	1.98	0.45
1:B:390:GLN:HG2	1:B:400:GLN:CD	2.42	0.44
1:A:159:PRO:HG2	1:A:254:VAL:HG22	1.99	0.44
1:B:167:ALA:C	1:B:218:ASP:HB2	2.43	0.44
1:A:207:ILE:HD12	1:A:207:ILE:H	1.83	0.44
1:B:155:ALA:O	1:B:254:VAL:HG22	2.17	0.44
1:A:132:GLN:NE2	1:A:373:GLU:OE2	2.50	0.44
1:B:272:GLN:HA	1:B:275:ILE:HG22	1.99	0.44
1:A:118:VAL:HG12	1:A:222:ILE:HG21	1.98	0.44
1:B:143:ARG:HG2	1:B:143:ARG:HH11	1.83	0.44
1:A:271:ARG:NH1	1:A:381:PHE:O	2.51	0.44
1:B:176:HIS:C	1:B:180:LEU:HD13	2.38	0.44
1:B:158:PHE:HB3	1:B:159:PRO:HD3	2.00	0.43
1:B:287:GLU:OE2	1:B:342:ARG:HD2	2.18	0.43
1:A:186:ARG:O	4:A:603:HOH:O	2.21	0.43
1:B:264:LEU:O	1:B:271:ARG:HD3	2.18	0.43
1:A:96:TYR:HD1	1:A:193:PHE:HZ	1.67	0.43
1:B:169:LEU:CB	1:B:170:PRO:CD	2.86	0.43
1:B:201:TYR:HB3	1:B:239:LYS:HD2	2.01	0.42
1:B:335:PRO:C	1:B:337:HIS:H	2.26	0.42
1:B:182:ASP:O	1:B:186:ARG:N	2.39	0.42
2:A:501:HEM:HBC2	2:A:501:HEM:HMC1	2.01	0.42
1:B:160:ILE:HG21	1:B:174:ILE:HG23	2.01	0.42
1:A:273:GLU:OE2	1:A:277:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ALA:C	1:B:193:PHE:HE2	2.27	0.42
1:A:127:LEU:HD21	1:A:165:LEU:HD21	2.02	0.42
1:B:214:LYS:HB3	1:B:214:LYS:HE3	1.34	0.42
1:B:291:ARG:NH2	1:B:336:MET:HE3	2.34	0.42
1:A:360:GLN:OE1	4:A:604:HOH:O	2.22	0.42
1:B:181:THR:HG22	1:B:251:ASP:HB3	2.02	0.42
1:B:156:GLU:HA	1:B:254:VAL:HG22	2.01	0.42
1:B:87:ARG:CD	1:B:92:ALA:HB1	2.41	0.41
1:B:332:ASN:ND2	1:B:346:SER:O	2.54	0.41
1:A:271:ARG:O	1:A:275:ILE:HG22	2.20	0.41
1:B:56:THR:O	1:B:61:GLY:HA2	2.21	0.41
1:B:204:LEU:HD23	1:B:204:LEU:HA	1.89	0.41
1:B:170:PRO:HB2	1:B:171:GLU:H	1.62	0.41
1:A:345:VAL:HG12	1:A:347:HIS:HD2	1.86	0.41
1:A:56:THR:O	1:A:61:GLY:HA2	2.21	0.40
1:B:203:TYR:O	1:B:206:PRO:HD2	2.22	0.40
1:A:277:ARG:NH2	1:A:280:ARG:CZ	2.84	0.40
1:A:287:GLU:OE2	1:A:342:ARG:HD2	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:733:HOH:O	4:B:734:HOH:O[1_655]	2.17	0.03
4:B:734:HOH:O	4:B:738:HOH:O[1_455]	2.18	0.02
4:A:687:HOH:O	4:A:721:HOH:O[1_455]	2.19	0.01

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	398/467 (85%)	387 (97%)	11 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	398/467 (85%)	382 (96%)	13 (3%)	3 (1%)	16	9
All	All	796/934 (85%)	769 (97%)	24 (3%)	3 (0%)	30	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	170	PRO
1	B	173	ASP
1	B	175	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	344/400 (86%)	342 (99%)	2 (1%)	78	83
1	B	341/400 (85%)	335 (98%)	6 (2%)	51	51
All	All	685/800 (86%)	677 (99%)	8 (1%)	63	65

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	LEU
1	A	222	ILE
1	B	152	GLU
1	B	174	ILE
1	B	197	LYS
1	B	207	ILE
1	B	211	ARG
1	B	336	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	59	ASN
1	A	227	GLN
1	A	311	GLN
1	A	343	GLN
1	B	116	ASN
1	B	225	ASN
1	B	311	GLN
1	B	332	ASN
1	B	390	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A1EI5	A	502	-	19,19,19	0.19	0	30,32,32	1.20	1 (3%)
3	A1EI5	B	502	-	19,19,19	0.21	0	30,32,32	1.18	1 (3%)
2	HEM	A	501	1,4	50,50,50	1.44	6 (12%)	66,82,82	1.26	9 (13%)
2	HEM	B	501	1,4	50,50,50	1.40	8 (16%)	66,82,82	1.25	9 (13%)

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	A1EI5	A	502	-	-	-	0/3/3/3
3	A1EI5	B	502	-	-	-	0/3/3/3
2	HEM	A	501	1,4	-	1/14/54/54	-
2	HEM	B	501	1,4	-	3/14/54/54	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	FE-NB	3.68	2.06	1.94
2	A	501	HEM	FE-NA	3.65	2.07	1.95
2	B	501	HEM	FE-NA	3.45	2.06	1.95
2	B	501	HEM	FE-ND	3.15	2.04	1.94
2	B	501	HEM	FE-NB	3.09	2.04	1.94
2	B	501	HEM	CAC-C3C	3.06	1.55	1.47
2	A	501	HEM	CAB-C3B	3.05	1.55	1.47
2	A	501	HEM	CAC-C3C	3.01	1.55	1.47
2	B	501	HEM	CAB-C3B	3.00	1.55	1.47
2	A	501	HEM	FE-NC	2.98	2.05	1.95
2	A	501	HEM	FE-ND	2.91	2.03	1.94
2	B	501	HEM	FE-NC	2.63	2.04	1.95
2	B	501	HEM	CMC-C2C	2.09	1.55	1.50
2	B	501	HEM	CMB-C2B	2.00	1.55	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	A1EI5	O1-C12-C16	-5.06	93.88	101.78
3	B	502	A1EI5	O1-C12-C16	-4.96	94.04	101.78
2	A	501	HEM	C4D-ND-C1D	3.34	108.52	105.07
2	B	501	HEM	C4D-ND-C1D	3.10	108.27	105.07
2	A	501	HEM	C4A-NA-C1A	2.93	108.21	105.35
2	B	501	HEM	C4C-NC-C1C	2.92	108.20	105.35
2	B	501	HEM	C4A-NA-C1A	2.70	107.99	105.35
2	A	501	HEM	C1B-NB-C4B	2.66	107.82	105.07
2	B	501	HEM	C1B-NB-C4B	2.63	107.78	105.07
2	A	501	HEM	C4C-NC-C1C	2.63	107.92	105.35
2	B	501	HEM	CAD-CBD-CGD	-2.51	108.21	113.60
2	A	501	HEM	C3B-C2B-C1B	2.28	108.17	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C3D-C4D-ND	-2.26	107.65	110.17
2	A	501	HEM	C2D-C1D-ND	-2.18	107.28	109.88
2	A	501	HEM	CAD-CBD-CGD	-2.17	108.93	113.60
2	B	501	HEM	C3D-C4D-ND	-2.12	107.81	110.17
2	B	501	HEM	C2D-C1D-ND	-2.05	107.42	109.88
2	B	501	HEM	C3B-C2B-C1B	2.05	108.01	106.49
2	A	501	HEM	C2A-C1A-NA	-2.05	107.86	110.15
2	B	501	HEM	C2A-C1A-NA	-2.04	107.86	110.15

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	HEM	CAA-CBA-CGA-O2A
2	B	501	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	CAD-CBD-CGD-O2D
2	B	501	HEM	CAD-CBD-CGD-O2D

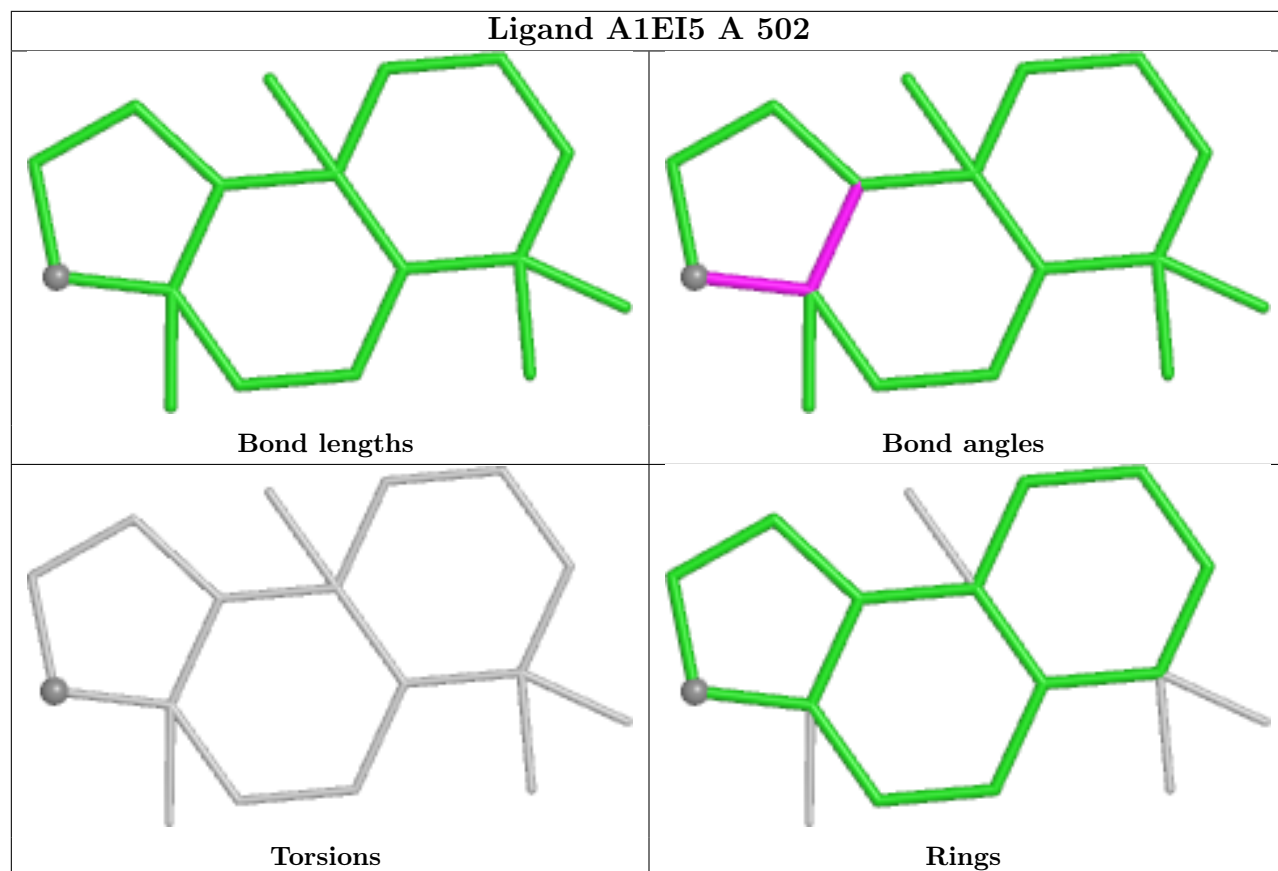
There are no ring outliers.

2 monomers are involved in 4 short contacts:

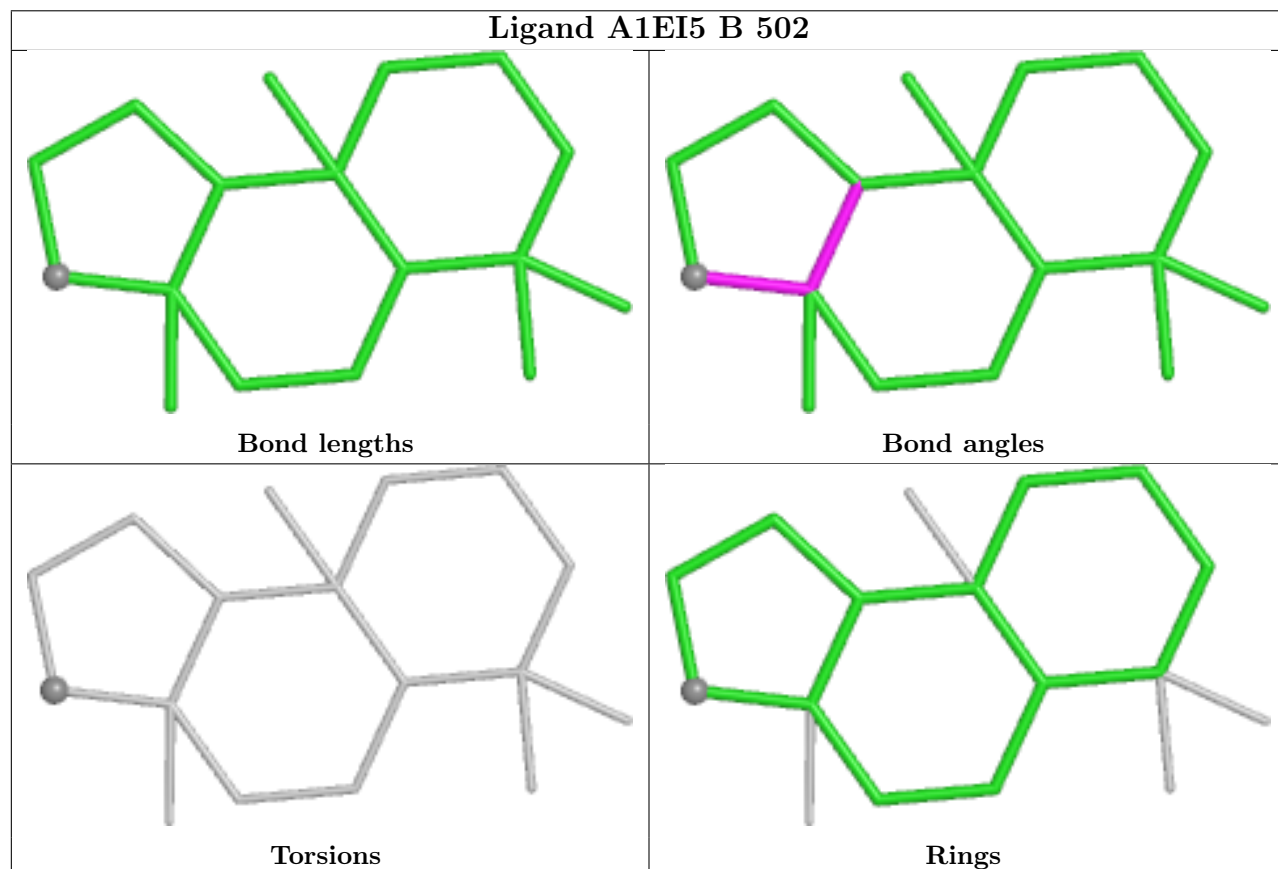
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	2	0
2	B	501	HEM	2	0

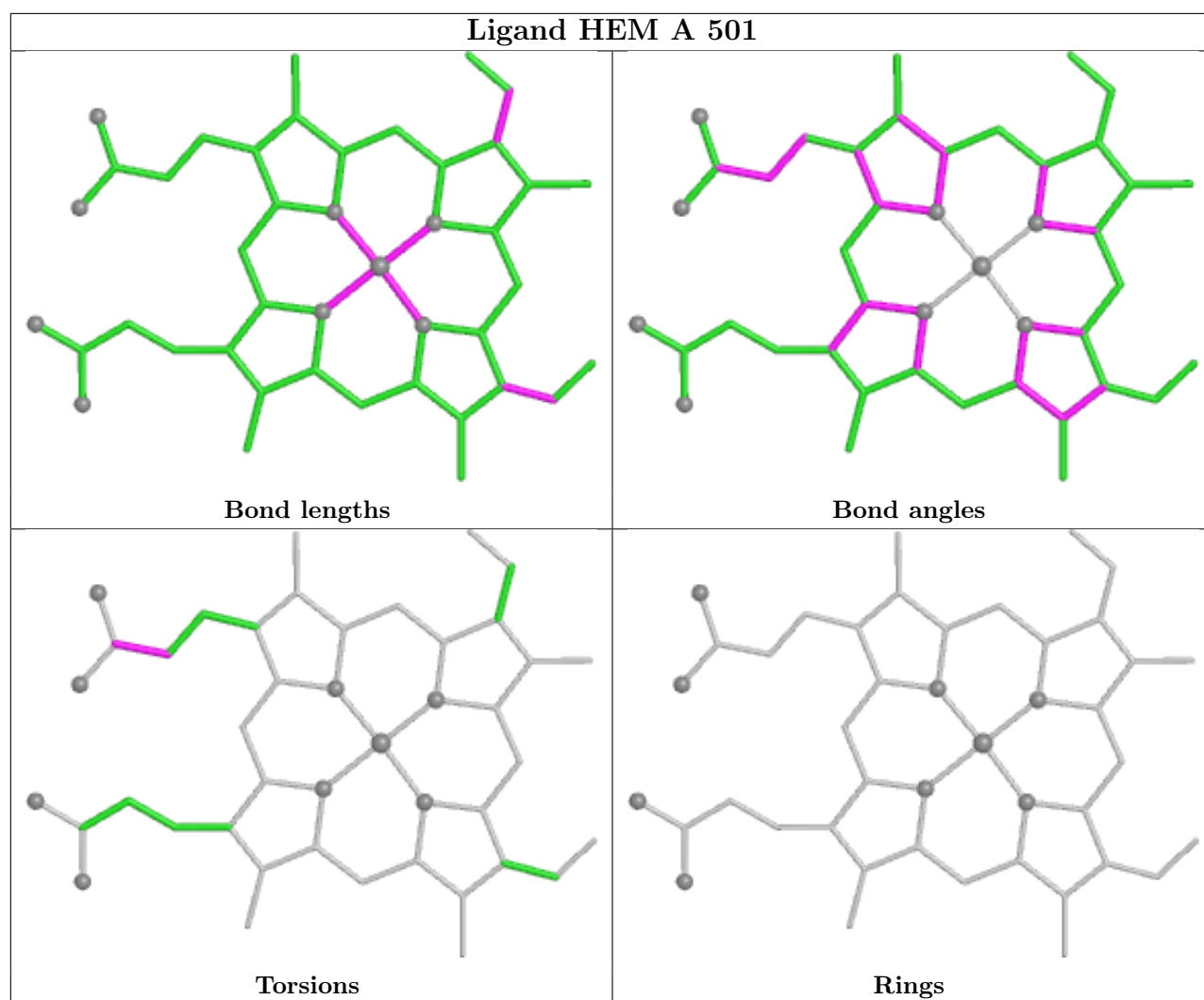
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

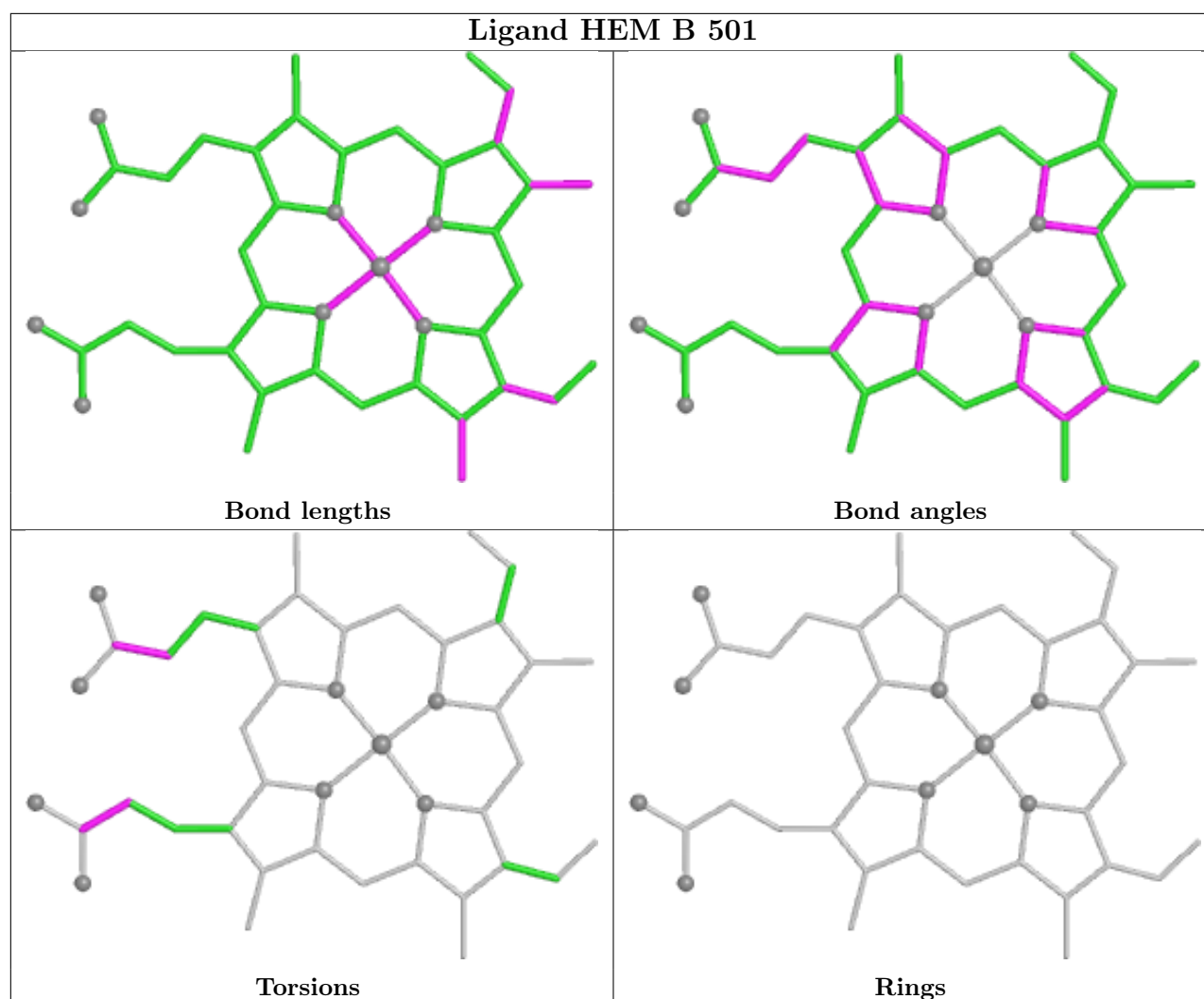
Ligand A1EI5 A 502



Ligand A1EI5 B 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	400/467 (85%)	0.66	19 (4%) 35 36	29, 45, 72, 90	0
1	B	400/467 (85%)	0.91	59 (14%) 5 5	25, 44, 93, 118	0
All	All	800/934 (85%)	0.79	78 (9%) 13 13	25, 45, 83, 118	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	173	ASP	8.5
1	B	177	LEU	7.7
1	B	179	TYR	6.3
1	B	175	PRO	6.2
1	B	172	GLU	6.0
1	B	170	PRO	5.6
1	B	180	LEU	5.2
1	B	193	PHE	5.1
1	B	174	ILE	5.1
1	B	96	TYR	5.0
1	B	183	GLN	4.9
1	B	184	MET	4.8
1	B	182	ASP	4.6
1	B	92	ALA	4.2
1	B	181	THR	4.2
1	B	335	PRO	4.2
1	A	409	ALA	4.1
1	B	191	MET	4.0
1	B	171	GLU	3.9
1	B	176	HIS	3.7
1	B	185	THR	3.6
1	B	10	ASN	3.6
1	B	93	GLY	3.6
1	B	336	MET	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	200	LEU	3.3
1	B	187	PRO	3.3
1	B	178	LYS	3.2
1	A	96	TYR	3.1
1	B	190	SER	3.1
1	B	199	ALA	3.1
1	B	189	GLY	3.1
1	A	384	ALA	3.0
1	B	196	ALA	3.0
1	B	192	THR	3.0
1	B	408	PRO	3.0
1	B	160	ILE	3.0
1	A	279	GLU	2.9
1	B	195	GLU	2.9
1	B	166	LEU	2.8
1	A	92	ALA	2.7
1	B	194	ALA	2.7
1	A	170	PRO	2.7
1	B	409	ALA	2.6
1	B	333	ALA	2.6
1	B	334	ALA	2.6
1	B	167	ALA	2.6
1	B	169	LEU	2.6
1	B	188	ASP	2.6
1	A	193	PHE	2.5
1	B	198	GLU	2.5
1	B	207	ILE	2.5
1	B	201	TYR	2.5
1	B	210	GLN	2.5
1	A	187	PRO	2.5
1	B	95	ALA	2.5
1	B	205	ILE	2.4
1	A	332	ASN	2.4
1	A	334	ALA	2.4
1	B	400	GLN	2.3
1	A	249	GLY	2.3
1	B	186	ARG	2.3
1	A	200	LEU	2.3
1	B	162	ILE	2.2
1	A	285	CYS	2.2
1	A	160	ILE	2.2
1	B	215	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	383	ILE	2.2
1	A	192	THR	2.2
1	B	247	VAL	2.1
1	B	87	ARG	2.1
1	A	91	GLU	2.1
1	B	246	LEU	2.1
1	A	275	ILE	2.1
1	B	219	ALA	2.1
1	A	165	LEU	2.1
1	B	250	LEU	2.1
1	A	167	ALA	2.1
1	B	230	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

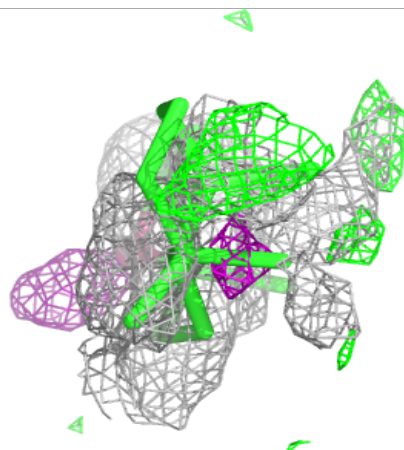
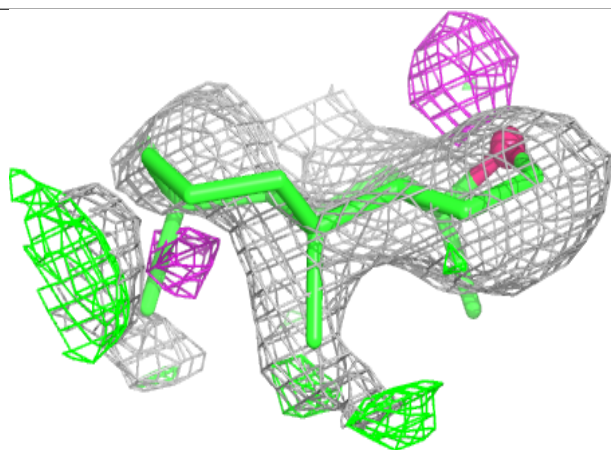
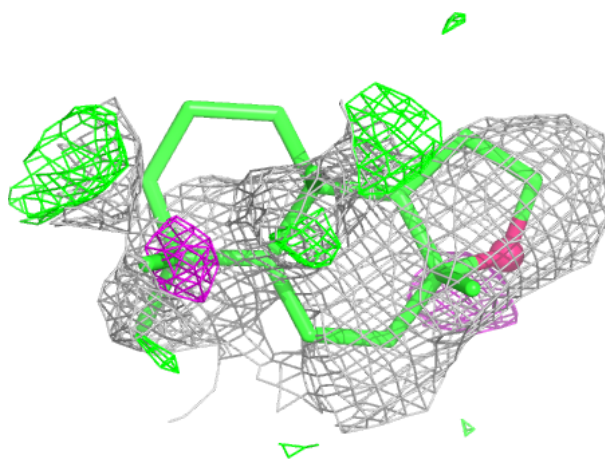
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	A1EI5	A	502	17/17	0.58	0.21	47,61,65,65	0
3	A1EI5	B	502	17/17	0.65	0.24	48,67,72,75	0
2	HEM	A	501	43/43	0.97	0.07	25,29,34,35	0
2	HEM	B	501	43/43	0.97	0.07	21,27,33,36	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.

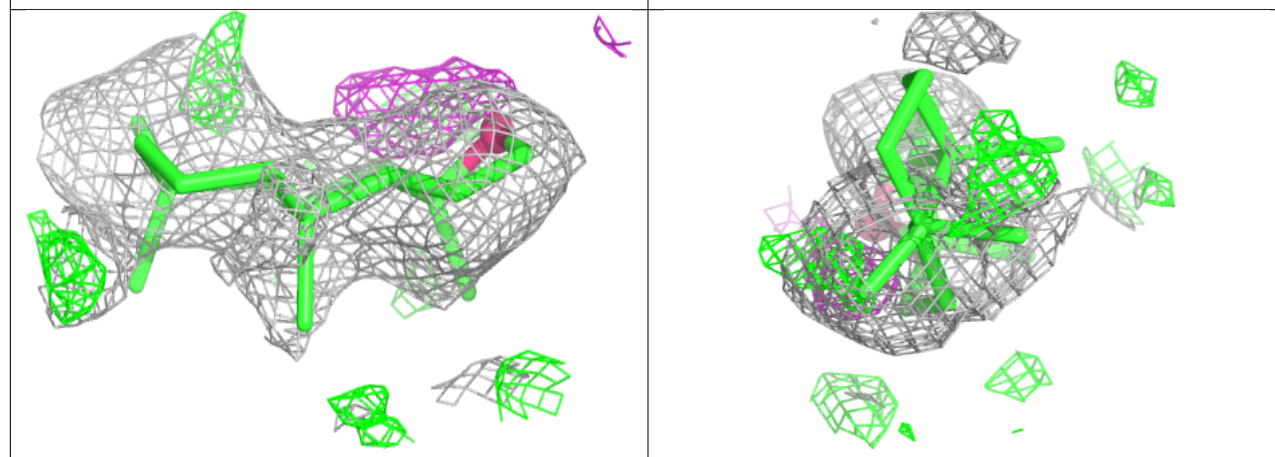
Electron density around A1EI5 A 502:

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



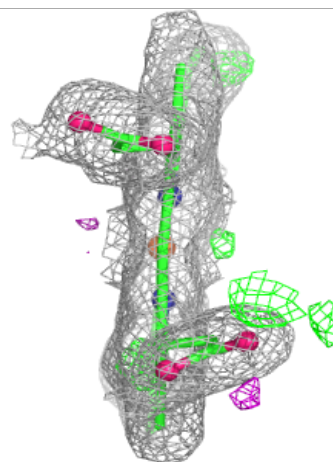
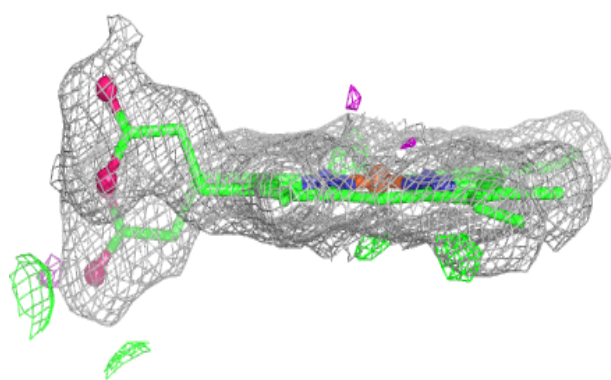
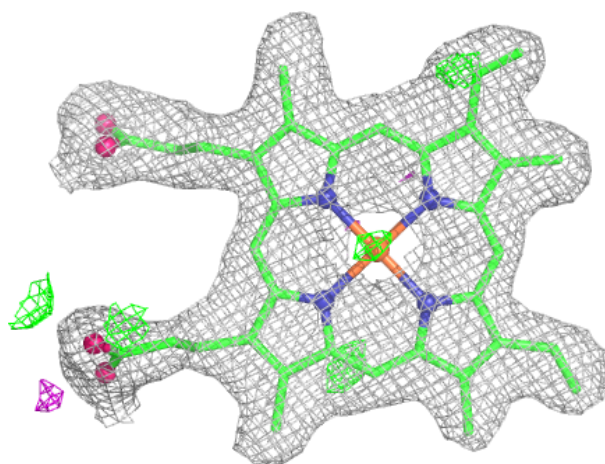
Electron density around A1EI5 B 502:

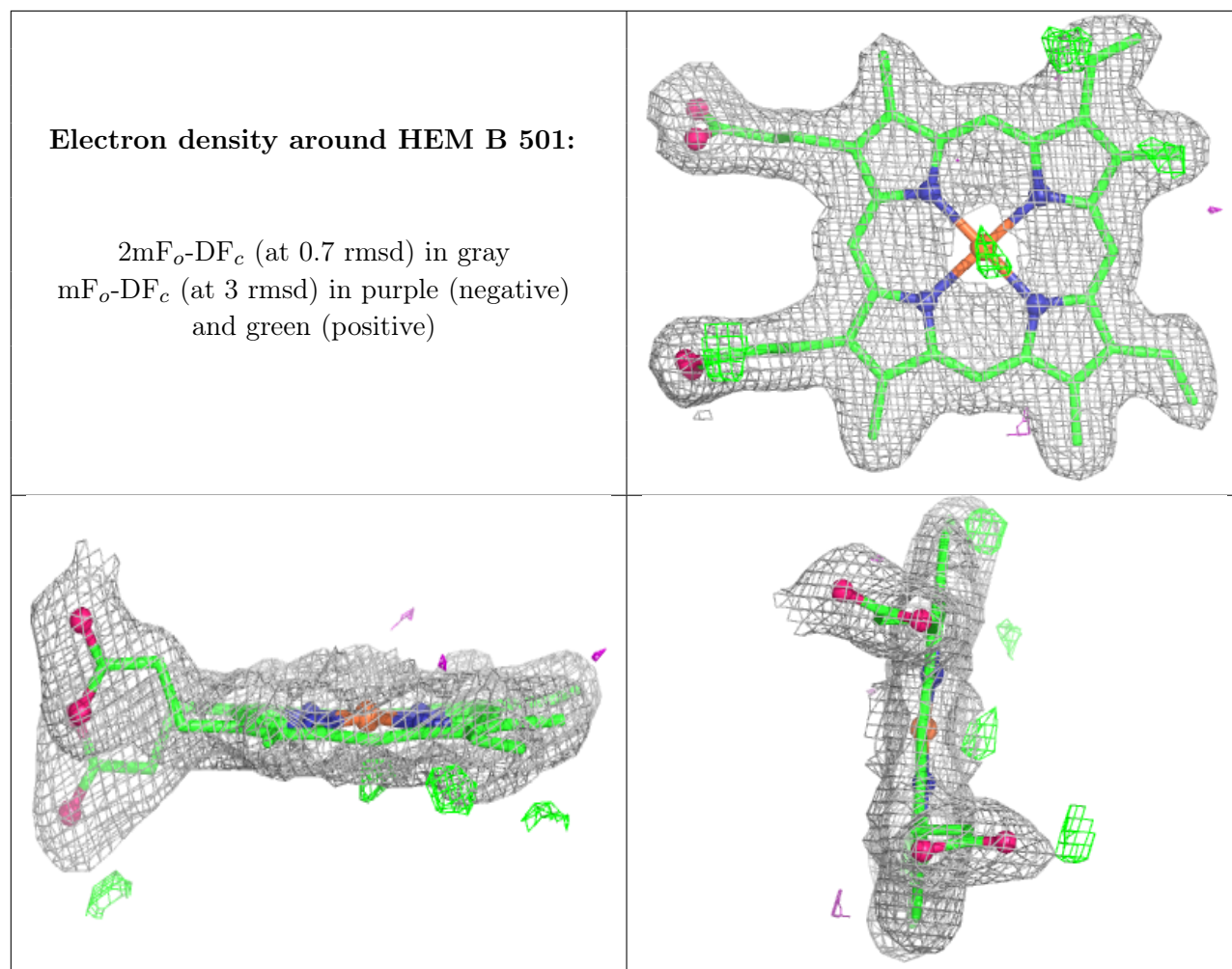
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.