



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:48 PM UTC

PDB ID : 7F3W / pdb_00007f3w
Title : Crystal structure of cytochrome P450DA mutant (N190F/V356L/A486E) heme domain
Authors : Wan, N.W.
Deposited on : 2021-06-17
Resolution : 2.86 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

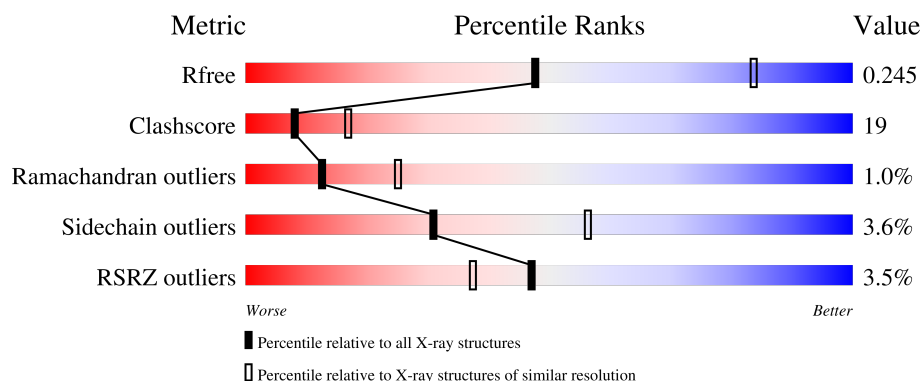
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	493	
1	B	493	
1	C	493	
1	D	493	

2 Entry composition [i](#)

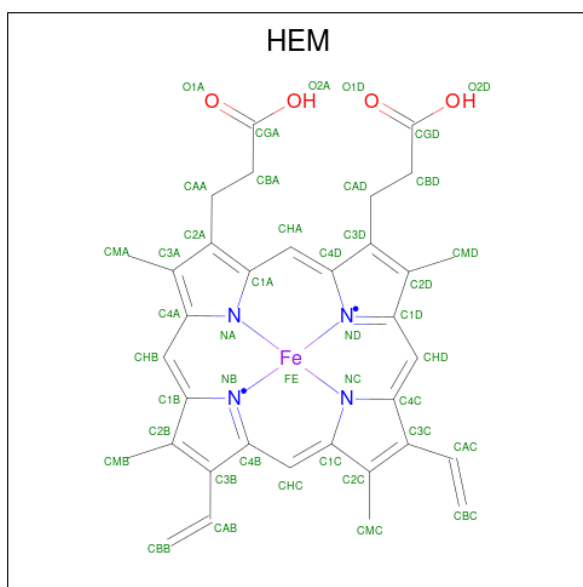
There are 3 unique types of molecules in this entry. The entry contains 15015 atoms, of which 120 are hydrogens and 0 are deuteriums.

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	464	Total	C	N	O	S	0	0	0
			3735	2381	670	671	13			
1	B	460	Total	C	N	O	S	0	0	0
			3702	2359	663	667	13			
1	C	454	Total	C	N	O	S	0	1	0
			3683	2349	659	662	13			
1	D	440	Total	C	N	O	S	0	0	0
			3553	2272	629	640	12			

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



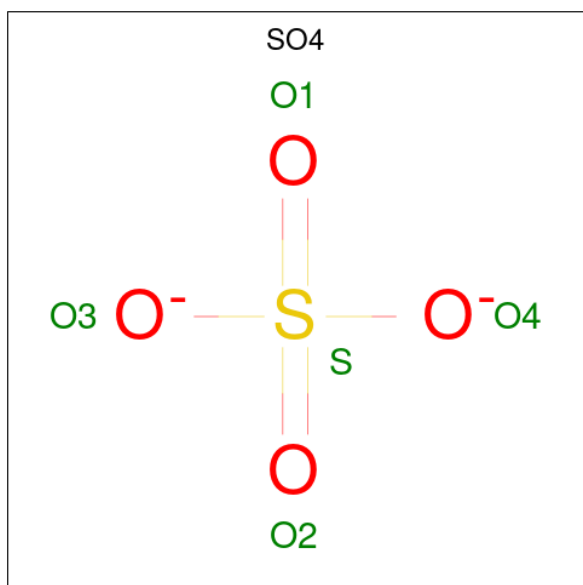
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	H	N O	0	0
			73	34	1	30	4 4		
2	B	1	Total	C	Fe	H	N O	0	0
			73	34	1	30	4 4		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	D	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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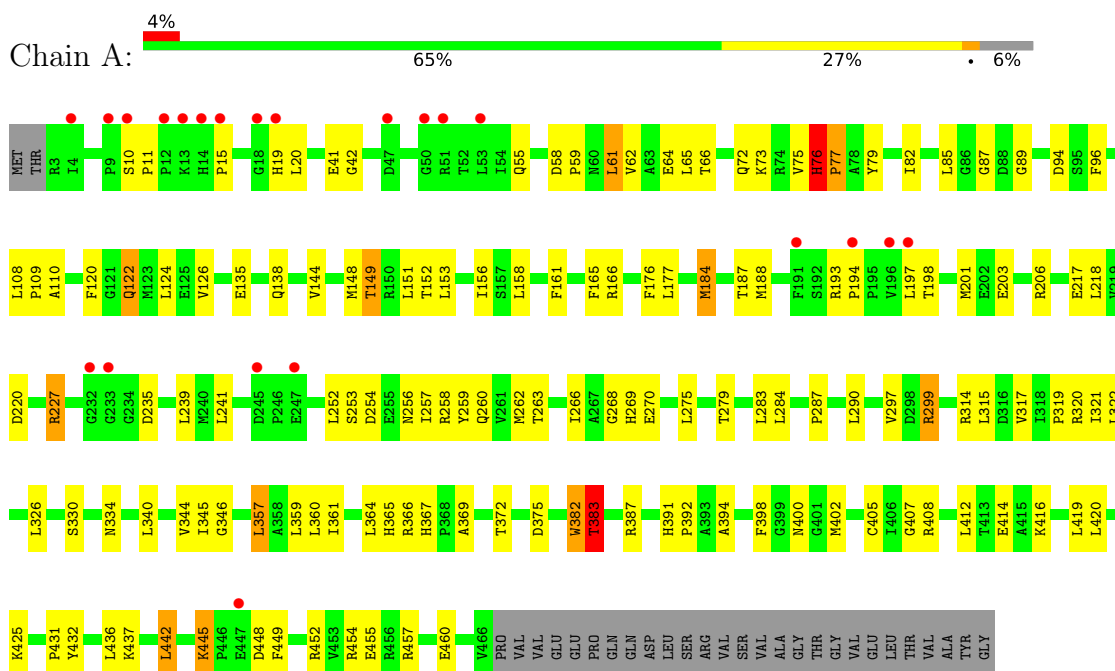
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		

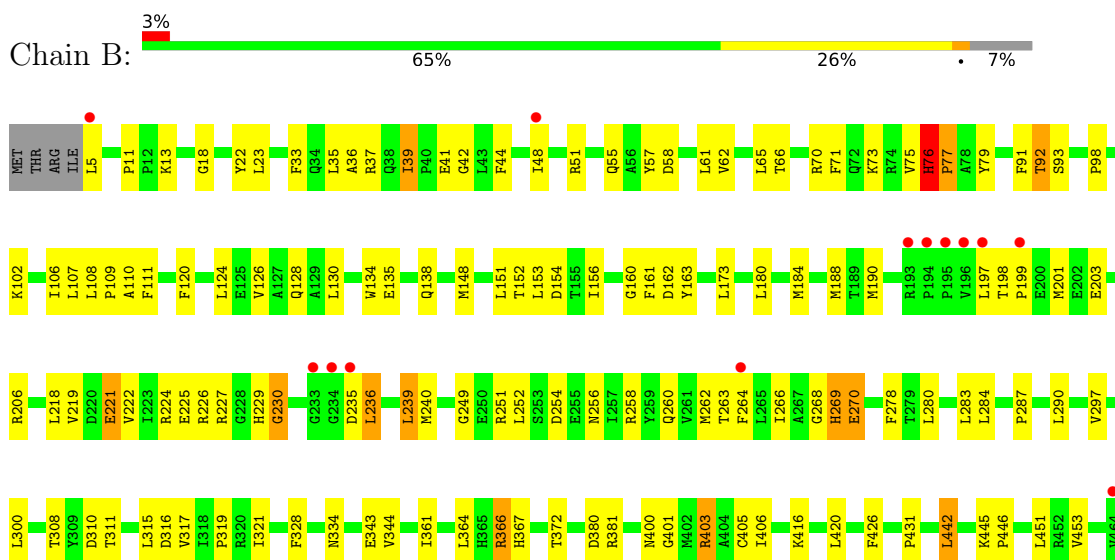
3 Residue-property plots

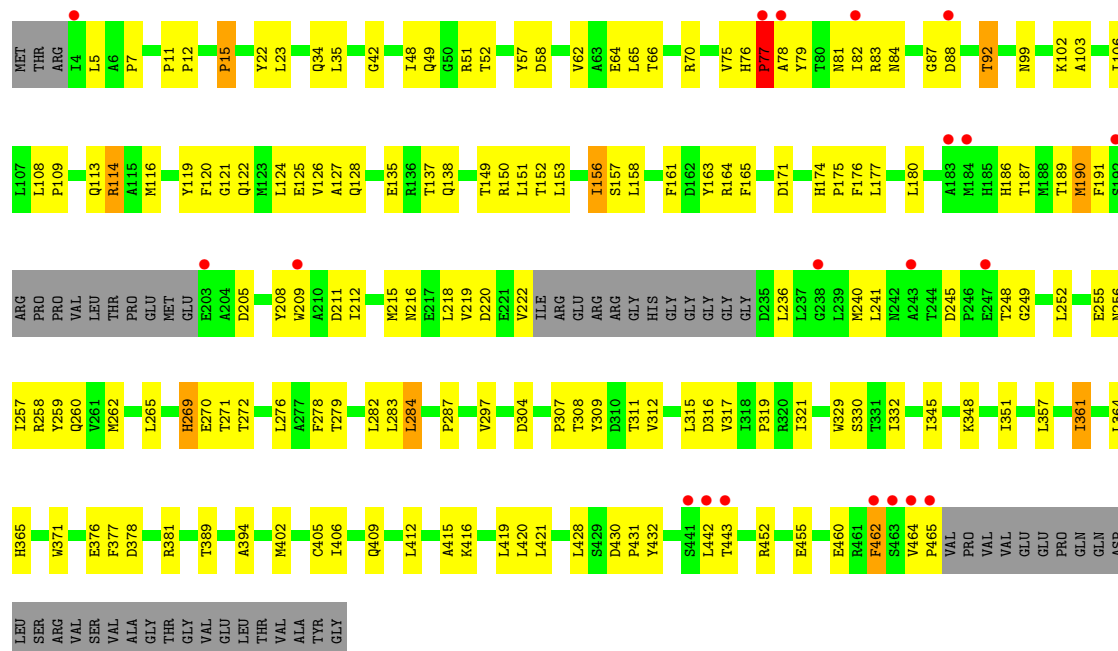
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



• Molecule 1: cytochrome P450





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	426.82Å 63.90Å 95.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.14 – 2.86 29.14 – 2.86	Depositor EDS
% Data completeness (in resolution range)	68.7 (29.14-2.86) 76.3 (29.14-2.86)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 2.85Å)	Xtriage
Refinement program	PHENIX 1.18.1_3865	Depositor
R, R_{free}	0.193 , 0.243 0.193 , 0.245	Depositor DCC
R_{free} test set	1998 reflections (3.21%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 30.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15015	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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

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	0.59	0/3832	0.91	12/5203 (0.2%)
1	B	0.53	1/3798 (0.0%)	0.77	3/5156 (0.1%)
1	C	0.53	1/3777 (0.0%)	0.78	2/5127 (0.0%)
1	D	0.51	1/3644 (0.0%)	0.78	5/4948 (0.1%)
All	All	0.54	3/15051 (0.0%)	0.81	22/20434 (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	A	0	1
1	B	0	1
1	C	0	2
1	D	0	2
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	373	ASN	C-O	-7.14	1.20	1.23
1	B	361	ILE	CA-CB	-6.43	1.50	1.54
1	D	361	ILE	CA-CB	6.43	1.57	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	383	THR	N-CA-C	-8.54	95.72	108.79
1	D	77	PRO	N-CA-CB	-8.41	94.42	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	PRO	N-CA-C	-6.94	103.88	113.53
1	B	442	LEU	N-CA-C	-6.72	104.03	111.36
1	A	442	LEU	N-CA-C	-6.71	104.05	111.36
1	C	189	THR	N-CA-C	-6.22	103.36	113.19
1	D	7	PRO	CA-C-N	-6.21	118.12	122.59
1	D	7	PRO	C-N-CA	-6.21	118.12	122.59
1	B	236	LEU	N-CA-C	6.12	117.62	111.07
1	C	361	ILE	CB-CA-C	-6.10	107.89	114.35
1	D	442	LEU	N-CA-C	-6.08	104.66	111.28
1	A	194	PRO	N-CA-C	-5.77	103.66	110.70
1	D	462	PHE	CA-CB-CG	5.75	119.55	113.80
1	A	19	HIS	N-CA-C	-5.74	106.28	113.28
1	A	227	ARG	N-CA-C	-5.71	105.19	111.82
1	A	268	GLY	CA-C-N	-5.54	109.84	121.80
1	A	268	GLY	C-N-CA	-5.54	109.84	121.80
1	A	448	ASP	CB-CA-C	5.35	121.07	110.42
1	A	445	LYS	N-CA-C	5.34	113.03	108.22
1	A	235	ASP	CA-CB-CG	5.30	117.90	112.60
1	B	239	LEU	N-CA-C	-5.13	105.58	111.07
1	A	382	TRP	CA-C-O	-5.05	115.28	120.54

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	76	HIS	Peptide
1	B	76	HIS	Peptide
1	C	462	PHE	Peptide
1	C	76	HIS	Peptide
1	D	114	ARG	Peptide
1	D	460	GLU	Mainchain

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	3735	0	3693	128	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3702	0	3652	131	0
1	C	3683	0	3642	144	0
1	D	3553	0	3506	171	0
2	A	43	30	30	5	0
2	B	43	30	30	5	0
2	C	43	30	30	6	0
2	D	43	30	30	10	0
3	A	10	0	0	1	0
3	B	15	0	0	0	0
3	C	15	0	0	0	0
3	D	10	0	0	1	0
All	All	14895	120	14613	575	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 19.

All (575) 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:85:LEU:HD11	1:A:266:ILE:HD11	1.32	1.09
1:A:85:LEU:HD11	1:A:266:ILE:CD1	1.82	1.09
1:A:85:LEU:CD1	1:A:266:ILE:HD11	1.93	0.98
1:D:283:LEU:HD21	1:D:321:ILE:HD13	1.43	0.97
1:D:332:ILE:HG13	1:D:443:THR:HG22	1.48	0.95
1:B:283:LEU:HD21	1:B:321:ILE:HD13	1.48	0.92
1:C:240:MET:HE2	1:C:257:ILE:HG23	1.52	0.91
1:B:227:ARG:NH1	1:B:254:ASP:OD1	2.04	0.90
1:D:88:ASP:OD2	1:D:99:ASN:ND2	2.05	0.90
1:D:332:ILE:CG1	1:D:443:THR:HG22	2.02	0.90
1:B:42:GLY:HA3	1:B:58:ASP:HB2	1.54	0.89
1:D:212:ILE:HG22	1:D:216:ASN:OD1	1.73	0.88
1:D:215:MET:HE3	1:D:262:MET:HE1	1.56	0.87
1:D:120:PHE:CE2	1:D:308:THR:HA	2.09	0.86
1:D:282:LEU:HD13	1:D:377:PHE:CE2	2.11	0.86
1:C:412:LEU:O	1:C:416:LYS:HG3	1.76	0.85
1:B:39:ILE:HG13	1:B:39:ILE:O	1.74	0.85
1:D:81:ASN:HD22	1:D:190:MET:HG3	1.41	0.85
1:B:297:VAL:HG22	1:B:420:LEU:HD12	1.58	0.85
2:C:501:HEM:HMC1	2:C:501:HEM:HBC2	1.58	0.84
1:B:110:ALA:HB2	1:B:239:LEU:HD22	1.59	0.84
1:D:187:THR:HA	1:D:190:MET:HE3	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:GLY:HA3	1:D:259:TYR:HD2	1.39	0.84
1:C:440:GLN:HB2	1:C:444:ILE:HG22	1.58	0.84
1:A:188:MET:HE3	1:A:442:LEU:HB2	1.60	0.84
1:D:87:GLY:HA3	1:D:259:TYR:CD2	2.12	0.84
1:A:299:ARG:HG3	1:A:299:ARG:HH11	1.42	0.84
2:A:501:HEM:HBB2	2:A:501:HEM:HMB1	1.58	0.83
1:D:282:LEU:HD13	1:D:377:PHE:HE2	1.44	0.82
1:B:70:ARG:HB3	1:B:343:GLU:OE2	1.79	0.82
1:D:120:PHE:HE2	1:D:308:THR:HA	1.41	0.81
1:D:284:LEU:HD13	1:D:430:ASP:HB2	1.60	0.81
1:B:22:TYR:CE1	1:B:35:LEU:HD22	2.16	0.81
1:D:240:MET:HE3	1:D:257:ILE:HG23	1.63	0.81
1:B:110:ALA:HB2	1:B:239:LEU:CD2	2.11	0.80
1:C:364:LEU:HD11	1:C:394:ALA:HA	1.62	0.80
1:B:11:PRO:HG2	1:B:35:LEU:HD21	1.65	0.79
1:D:284:LEU:CD1	1:D:430:ASP:HB2	2.14	0.78
1:A:82:ILE:HD11	1:A:184:MET:HE1	1.65	0.78
1:A:153:LEU:HD23	1:A:177:LEU:HD13	1.65	0.78
1:A:73:LYS:HE3	1:A:79:TYR:CZ	2.20	0.77
1:A:82:ILE:CD1	1:A:184:MET:HE1	2.13	0.77
1:D:218:LEU:O	1:D:222:VAL:HG23	1.84	0.77
1:B:188:MET:HE3	1:B:442:LEU:HB2	1.64	0.77
1:C:240:MET:CE	1:C:257:ILE:HA	2.16	0.76
1:D:297:VAL:HG22	1:D:420:LEU:HD12	1.69	0.75
1:A:152:THR:O	1:A:156:ILE:HD12	1.86	0.75
1:A:454:ARG:NH2	1:D:377:PHE:O	2.20	0.75
1:D:255:GLU:HG2	1:D:259:TYR:CE1	2.22	0.75
1:C:316:ASP:C	1:C:319:PRO:HD2	2.12	0.74
1:D:216:ASN:HB3	1:D:258:ARG:NH1	2.02	0.74
1:A:66:THR:HG23	1:A:400:ASN:HD21	1.53	0.73
1:A:253:SER:O	1:A:257:ILE:HG13	1.88	0.73
1:B:66:THR:HG23	1:B:400:ASN:HD21	1.52	0.73
1:A:66:THR:HG23	1:A:400:ASN:ND2	2.04	0.72
1:C:83:ARG:NH2	1:C:97:GLU:OE2	2.22	0.72
1:C:198:THR:OG1	1:C:201:MET:HG2	1.90	0.71
1:C:126:VAL:HG12	1:C:151:LEU:HD12	1.72	0.71
1:C:11:PRO:HD2	1:C:19:HIS:CE1	2.24	0.71
1:D:271:THR:CG2	1:D:443:THR:HG21	2.21	0.71
1:B:161:PHE:CE1	1:B:163:TYR:HB2	2.25	0.71
1:B:62:VAL:HG21	1:B:364:LEU:HD13	1.73	0.71
1:C:219:VAL:O	1:C:223:ILE:HG12	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:LEU:HA	1:A:201:MET:HE2	1.74	0.70
1:B:161:PHE:CD1	1:B:163:TYR:HB2	2.26	0.70
1:C:316:ASP:O	1:C:319:PRO:HD2	1.91	0.70
1:B:300:LEU:HD12	1:B:315:LEU:HD12	1.74	0.69
1:C:22:TYR:CE1	1:C:35:LEU:HD11	2.28	0.69
1:B:161:PHE:CE1	1:B:163:TYR:CB	2.76	0.69
1:D:271:THR:HG22	1:D:443:THR:HG21	1.75	0.69
1:D:297:VAL:HG22	1:D:420:LEU:CD1	2.23	0.69
1:A:405:CYS:HB2	2:A:501:HEM:NA	2.08	0.69
1:D:209:TRP:HA	1:D:212:ILE:HD12	1.74	0.69
1:C:182:ARG:HH21	1:C:211:ASP:CG	2.01	0.68
1:D:138:GLN:OE1	1:D:455:GLU:HG3	1.93	0.68
1:A:85:LEU:HD11	1:A:266:ILE:HD12	1.73	0.67
1:A:299:ARG:HG3	1:A:299:ARG:NH1	2.06	0.67
1:C:152:THR:O	1:C:156:ILE:HG12	1.94	0.67
1:B:180:LEU:HD11	1:B:266:ILE:CD1	2.23	0.67
1:B:33:PHE:CZ	1:B:366:ARG:HD2	2.29	0.67
1:B:319:PRO:HG3	1:B:416:LYS:HE3	1.76	0.67
1:C:422:ILE:HG22	1:C:423:LEU:HD23	1.76	0.66
1:D:176:PHE:CE2	1:D:215:MET:HB3	2.30	0.66
1:B:405:CYS:HB2	2:B:501:HEM:NA	2.11	0.66
1:D:114:ARG:O	1:D:114:ARG:HG3	1.95	0.66
1:C:440:GLN:CB	1:C:444:ILE:HG22	2.25	0.65
1:C:240:MET:HE1	1:C:260:GLN:HB2	1.78	0.65
1:D:215:MET:HE3	1:D:262:MET:CE	2.24	0.65
1:C:198:THR:OG1	1:C:201:MET:CG	2.45	0.65
1:C:227:ARG:HE	1:C:241:LEU:HD22	1.62	0.65
1:B:218:LEU:O	1:B:222:VAL:HG23	1.97	0.65
1:C:418:ALA:O	1:C:422:ILE:HD12	1.97	0.65
2:C:501:HEM:HBB2	2:C:501:HEM:HMB2	1.79	0.65
1:B:107:LEU:HD13	1:B:264:PHE:HZ	1.62	0.64
1:D:103:ALA:HB1	1:D:260:GLN:HE21	1.62	0.64
1:C:81:ASN:O	1:C:84:ASN:HB2	1.96	0.64
1:C:76:HIS:CG	1:C:77:PRO:HD3	2.32	0.64
1:C:332:ILE:HD12	2:C:501:HEM:CHB	2.28	0.64
1:D:23:LEU:HD11	1:D:48:ILE:HG21	1.79	0.64
1:D:412:LEU:O	1:D:416:LYS:HG3	1.97	0.64
1:C:132:GLY:O	1:C:136:ARG:HG3	1.98	0.63
1:C:218:LEU:O	1:C:222:VAL:HG23	1.98	0.63
1:D:211:ASP:O	1:D:215:MET:HG3	1.98	0.63
1:B:162:ASP:HB3	1:B:226:ARG:HH12	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:VAL:HG21	1:A:364:LEU:HD13	1.81	0.63
1:A:87:GLY:HA3	1:A:259:TYR:CD1	2.34	0.63
1:D:135:GLU:O	1:D:138:GLN:HG3	1.98	0.63
1:B:102:LYS:O	1:B:106:ILE:HD12	1.99	0.63
1:B:184:MET:SD	1:B:266:ILE:HD12	2.39	0.62
2:C:501:HEM:HBC2	2:C:501:HEM:CMC	2.28	0.62
1:A:138:GLN:NE2	1:A:455:GLU:HG3	2.14	0.62
1:D:81:ASN:ND2	1:D:190:MET:HG3	2.14	0.62
1:A:59:PRO:HB2	1:A:391:HIS:CD2	2.34	0.62
1:C:55:GLN:HE22	1:C:334:ASN:HD21	1.47	0.62
1:D:332:ILE:HG12	1:D:443:THR:HG22	1.82	0.62
1:C:160:GLY:HA2	1:C:236:LEU:HB2	1.82	0.62
2:B:501:HEM:HBB2	2:B:501:HEM:CMB	2.30	0.62
1:C:372:THR:O	1:C:381:ARG:NH2	2.32	0.62
1:B:66:THR:HA	1:B:400:ASN:ND2	2.14	0.62
2:D:501:HEM:HBC2	2:D:501:HEM:HMC2	1.80	0.62
1:D:124:LEU:HD21	1:D:128:GLN:NE2	2.15	0.61
1:D:220:ASP:OD1	1:D:258:ARG:HD3	1.99	0.61
1:A:89:GLY:HA2	1:A:260:GLN:NE2	2.15	0.61
1:B:130:LEU:HD11	1:B:134:TRP:CE2	2.35	0.61
1:B:262:MET:O	1:B:266:ILE:HG12	2.01	0.61
1:C:402:MET:HE2	1:C:402:MET:HA	1.81	0.61
1:C:359:LEU:N	1:C:359:LEU:HD12	2.15	0.61
1:D:208:TYR:O	1:D:212:ILE:HD12	2.00	0.61
1:A:326:LEU:O	1:A:330:SER:OG	2.14	0.61
1:A:76:HIS:CD2	1:A:77:PRO:HD3	2.36	0.61
1:D:106:ILE:HD12	1:D:252:LEU:HG	1.83	0.61
1:D:127:ALA:HB1	1:D:421:LEU:HD12	1.83	0.60
1:C:161:PHE:CD2	1:C:261:VAL:HG13	2.35	0.60
1:A:138:GLN:HE22	1:A:455:GLU:HG3	1.67	0.60
1:A:402:MET:HE3	1:A:402:MET:HA	1.83	0.60
1:D:283:LEU:HD21	1:D:321:ILE:CD1	2.24	0.60
1:C:284:LEU:HD13	1:C:430:ASP:HB2	1.85	0.59
1:B:156:ILE:HD11	1:B:264:PHE:HB3	1.85	0.59
1:C:281:TYR:CE2	1:C:436:LEU:HD22	2.37	0.59
1:D:65:LEU:HD21	1:D:357:LEU:HD22	1.84	0.59
1:A:41:GLU:OE1	1:A:41:GLU:N	2.30	0.59
1:B:198:THR:HB	1:B:199:PRO:HD2	1.84	0.59
1:C:351:ILE:HG23	1:C:355:GLN:HG2	1.85	0.59
1:B:73:LYS:HE3	1:B:79:TYR:CZ	2.38	0.59
1:B:240:MET:HE1	1:B:260:GLN:HB2	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLN:OE1	1:A:360:LEU:HD13	2.03	0.58
1:D:156:ILE:CG2	1:D:265:LEU:HD23	2.33	0.58
1:D:330:SER:OG	1:D:365:HIS:CE1	2.56	0.58
1:A:412:LEU:O	1:A:416:LYS:HG3	2.03	0.58
1:B:55:GLN:HE22	1:B:334:ASN:HD21	1.52	0.58
1:C:150:ARG:NH2	1:C:171:ASP:O	2.36	0.58
1:A:262:MET:O	1:A:266:ILE:HG12	2.03	0.58
1:D:212:ILE:HA	1:D:215:MET:HE2	1.85	0.58
1:A:66:THR:HG23	1:A:400:ASN:CG	2.28	0.58
1:B:252:LEU:HD22	1:B:256:ASN:OD1	2.02	0.58
1:A:320:ARG:HD2	1:A:382:TRP:O	2.04	0.58
1:D:88:ASP:CG	1:D:256:ASN:HD22	2.10	0.58
1:C:48:ILE:HG13	1:C:48:ILE:O	2.04	0.58
1:D:255:GLU:O	1:D:259:TYR:HD1	1.87	0.57
2:D:501:HEM:HBB2	2:D:501:HEM:HMB2	1.84	0.57
1:B:227:ARG:NH1	1:B:254:ASP:CG	2.61	0.57
1:C:161:PHE:CE1	1:C:163:TYR:HB2	2.39	0.57
1:A:454:ARG:HH22	1:D:377:PHE:C	2.12	0.57
1:A:364:LEU:HD21	1:A:394:ALA:HA	1.87	0.56
1:C:174:HIS:ND1	1:C:175:PRO:HD2	2.20	0.56
1:C:122:GLN:HG2	1:C:158:LEU:HG	1.86	0.56
1:C:126:VAL:CG1	1:C:151:LEU:HD12	2.36	0.56
1:D:153:LEU:O	1:D:156:ILE:HG22	2.05	0.56
1:D:364:LEU:HD11	1:D:394:ALA:HA	1.87	0.56
1:D:315:LEU:HD11	1:D:420:LEU:HD22	1.87	0.56
2:C:501:HEM:HBB2	2:C:501:HEM:CMB	2.35	0.56
1:B:229:HIS:O	1:B:230:GLY:C	2.48	0.56
1:B:11:PRO:CG	1:B:35:LEU:HD21	2.33	0.56
1:A:184:MET:CE	1:A:266:ILE:HD12	2.36	0.56
1:B:206:ARG:HB3	1:D:34:GLN:HG3	1.88	0.55
1:B:130:LEU:HD12	1:B:130:LEU:O	2.05	0.55
1:B:262:MET:HE2	1:B:262:MET:HA	1.88	0.55
1:C:409:GLN:O	1:C:413:THR:HG23	2.06	0.55
1:A:270:GLU:HG2	1:A:445:LYS:HE3	1.87	0.55
1:C:137:THR:O	1:C:140:GLN:HB2	2.06	0.55
1:A:319:PRO:HG3	1:A:416:LYS:HD3	1.88	0.55
1:B:372:THR:O	1:B:381:ARG:NH2	2.40	0.55
1:A:66:THR:HG23	1:A:400:ASN:OD1	2.06	0.55
1:B:426:PHE:HB3	1:B:453:VAL:HB	1.89	0.55
1:D:190:MET:HG3	1:D:190:MET:O	2.05	0.55
1:A:436:LEU:HD12	1:A:437:LYS:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:ARG:NH2	1:B:366:ARG:O	2.40	0.55
1:B:66:THR:HG23	1:B:400:ASN:ND2	2.21	0.55
1:D:76:HIS:O	1:D:77:PRO:C	2.50	0.55
1:C:275:LEU:HD21	1:C:322:LEU:HD22	1.89	0.55
1:A:317:VAL:O	1:A:321:ILE:HG13	2.07	0.55
1:A:59:PRO:CB	1:A:391:HIS:CD2	2.89	0.54
1:A:283:LEU:HB3	1:A:290:LEU:HB2	1.88	0.54
1:C:48:ILE:O	1:C:49:GLN:C	2.50	0.54
1:A:152:THR:HA	1:A:414:GLU:OE1	2.07	0.54
1:D:157:SER:HG	1:D:165:PHE:HE2	1.54	0.54
1:B:36:ALA:HB1	1:B:57:TYR:CZ	2.42	0.54
1:D:122:GLN:HB3	1:D:158:LEU:HD23	1.89	0.54
1:D:174:HIS:HD2	1:D:176:PHE:HB3	1.73	0.54
1:D:279:THR:HG21	1:D:419:LEU:HD11	1.90	0.54
1:B:400:ASN:OD1	1:B:401:GLY:N	2.41	0.54
1:D:42:GLY:HA2	1:D:57:TYR:CE1	2.42	0.54
1:A:454:ARG:HH21	1:D:376:GLU:HG2	1.72	0.54
1:B:66:THR:HA	1:B:400:ASN:HD21	1.73	0.54
1:D:137:THR:O	1:D:137:THR:HG22	2.08	0.54
1:D:255:GLU:HG2	1:D:259:TYR:HE1	1.68	0.54
2:D:501:HEM:HBB2	2:D:501:HEM:CMB	2.36	0.54
1:C:156:ILE:HD13	1:C:410:PHE:HE2	1.73	0.54
1:C:357:LEU:N	1:C:357:LEU:HD12	2.23	0.54
1:D:65:LEU:HD21	1:D:357:LEU:CD2	2.38	0.54
1:A:218:LEU:HD12	1:A:218:LEU:O	2.08	0.53
1:A:432:TYR:HA	3:A:503:SO4:O2	2.08	0.53
1:A:436:LEU:HD12	1:A:437:LYS:H	1.72	0.53
1:B:219:VAL:HG21	1:B:262:MET:HE3	1.89	0.53
1:D:316:ASP:C	1:D:319:PRO:HD2	2.33	0.53
1:B:148:MET:O	1:B:152:THR:HG23	2.09	0.53
1:C:85:LEU:C	1:C:85:LEU:HD12	2.33	0.53
1:C:58:ASP:O	1:C:62:VAL:HG23	2.07	0.53
1:D:156:ILE:HG23	1:D:265:LEU:HD23	1.89	0.53
1:B:58:ASP:HB3	1:B:61:LEU:HD12	1.90	0.53
1:C:351:ILE:CG2	1:C:355:GLN:HB3	2.38	0.53
1:B:110:ALA:CB	1:B:239:LEU:CD2	2.85	0.53
1:D:102:LYS:HA	1:D:245:ASP:OD2	2.08	0.53
1:C:345:ILE:HG12	1:C:351:ILE:HD11	1.91	0.53
1:A:85:LEU:HD13	1:A:266:ILE:HD11	1.86	0.53
1:A:203:GLU:HG3	1:A:206:ARG:HH21	1.74	0.52
1:A:290:LEU:HD23	1:D:287:PRO:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:THR:CG2	1:B:400:ASN:HD21	2.21	0.52
1:D:215:MET:CE	1:D:262:MET:HE1	2.35	0.52
1:A:206:ARG:HD2	1:C:34:GLN:HG3	1.90	0.52
1:B:197:LEU:HD23	1:B:201:MET:HE3	1.91	0.52
1:D:62:VAL:O	1:D:66:THR:HG23	2.09	0.52
1:D:65:LEU:HD21	1:D:357:LEU:CB	2.38	0.52
1:D:219:VAL:CG1	1:D:258:ARG:HG3	2.40	0.52
1:D:269:HIS:CE1	1:D:270:GLU:HG3	2.44	0.52
1:C:306:VAL:HG13	1:C:307:PRO:HD2	1.89	0.52
1:C:76:HIS:CG	1:C:77:PRO:CD	2.92	0.52
1:A:279:THR:HG21	1:A:419:LEU:HD11	1.92	0.52
1:B:126:VAL:HG12	1:B:151:LEU:HD12	1.91	0.52
1:D:81:ASN:HD22	1:D:190:MET:CG	2.19	0.52
1:D:108:LEU:CB	1:D:109:PRO:HD3	2.40	0.52
1:D:180:LEU:O	1:D:180:LEU:HD12	2.10	0.52
1:A:252:LEU:HD22	1:A:256:ASN:OD1	2.10	0.52
1:D:205:ASP:O	1:D:209:TRP:HD1	1.93	0.52
1:D:271:THR:HG23	1:D:443:THR:HG21	1.92	0.52
1:A:144:VAL:O	1:A:148:MET:HG2	2.09	0.52
1:B:160:GLY:HA2	1:B:236:LEU:HB2	1.92	0.52
1:C:383:THR:O	1:C:387[A]:ARG:HB2	2.10	0.52
1:D:315:LEU:HB3	1:D:319:PRO:HD3	1.91	0.52
1:C:212:ILE:HA	1:C:215:MET:HE3	1.91	0.52
1:A:359:LEU:CD1	1:A:359:LEU:N	2.72	0.51
1:A:184:MET:HA	1:A:184:MET:HE2	1.92	0.51
1:C:14:HIS:HB2	1:C:21:HIS:CE1	2.46	0.51
1:B:316:ASP:C	1:B:319:PRO:HD2	2.36	0.51
1:D:190:MET:HE1	1:D:208:TYR:CE2	2.45	0.51
1:C:221:GLU:O	1:C:221:GLU:HG3	2.09	0.51
1:D:240:MET:CE	1:D:257:ILE:HG23	2.36	0.51
1:B:124:LEU:HD12	1:B:128:GLN:HG3	1.92	0.51
1:C:78:ALA:HB3	1:C:79:TYR:CD1	2.44	0.51
1:D:330:SER:OG	1:D:365:HIS:HE1	1.93	0.51
1:B:152:THR:OG1	1:B:269:HIS:HA	2.10	0.51
2:B:501:HEM:HBB2	2:B:501:HEM:HMB2	1.92	0.51
1:C:76:HIS:CD2	1:C:77:PRO:HD3	2.45	0.51
1:C:220:ASP:OD1	1:C:258:ARG:HD3	2.11	0.51
1:D:75:VAL:HG13	1:D:79:TYR:HB2	1.93	0.51
1:D:102:LYS:HE3	1:D:252:LEU:HD23	1.93	0.51
1:A:203:GLU:OE2	1:A:206:ARG:NH2	2.44	0.50
1:D:462:PHE:HB3	1:D:464:VAL:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:GLU:OE2	1:D:345:ILE:HA	2.11	0.50
1:D:409:GLN:H	1:D:409:GLN:NE2	2.09	0.50
1:A:79:TYR:OH	2:A:501:HEM:O2A	2.18	0.50
1:B:66:THR:CA	1:B:400:ASN:HD21	2.25	0.50
1:C:441:SER:OG	1:C:442:LEU:N	2.44	0.50
1:B:98:PRO:O	1:B:102:LYS:HG3	2.12	0.50
1:A:110:ALA:HB2	1:A:239:LEU:HD13	1.94	0.50
1:D:119:TYR:CE1	1:D:236:LEU:CD2	2.95	0.50
1:A:110:ALA:HB2	1:A:239:LEU:CD1	2.41	0.50
1:B:180:LEU:HD11	1:B:266:ILE:HD11	1.91	0.50
1:C:215:MET:O	1:C:219:VAL:HG23	2.11	0.50
1:D:124:LEU:HD21	1:D:128:GLN:HE22	1.76	0.50
1:D:405:CYS:HB2	2:D:501:HEM:NA	2.26	0.50
1:A:284:LEU:HD23	1:D:287:PRO:HG3	1.92	0.50
1:D:103:ALA:CB	1:D:260:GLN:HE21	2.25	0.50
1:D:120:PHE:CE2	1:D:308:THR:CA	2.90	0.50
1:D:150:ARG:NH2	1:D:171:ASP:O	2.44	0.50
1:A:284:LEU:HD12	1:A:449:PHE:HZ	1.76	0.49
1:A:359:LEU:N	1:A:359:LEU:HD12	2.26	0.49
1:D:260:GLN:OE1	1:D:260:GLN:HA	2.12	0.49
1:B:37:ARG:HH22	1:B:367:HIS:HA	1.77	0.49
1:B:311:THR:O	1:B:315:LEU:HD13	2.11	0.49
1:B:451:LEU:HD12	1:B:451:LEU:C	2.37	0.49
1:D:106:ILE:CD1	1:D:252:LEU:HG	2.42	0.49
1:D:161:PHE:CE2	1:D:163:TYR:HB2	2.47	0.49
1:D:271:THR:HB	2:D:501:HEM:C3B	2.47	0.49
1:C:37:ARG:HH21	1:C:366:ARG:HB3	1.77	0.49
1:A:256:ASN:O	1:A:260:GLN:HG2	2.12	0.49
1:B:111:PHE:HB3	1:B:406:ILE:O	2.13	0.49
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.43	0.49
1:C:130:LEU:HD12	1:C:168:PHE:CE1	2.47	0.49
1:D:186:HIS:ND1	1:D:190:MET:HE2	2.28	0.49
1:A:66:THR:HG22	1:A:66:THR:O	2.13	0.49
1:C:161:PHE:CD2	1:C:261:VAL:CG1	2.96	0.49
1:C:161:PHE:CD1	1:C:163:TYR:HB2	2.48	0.49
1:D:103:ALA:HB1	1:D:260:GLN:NE2	2.27	0.49
1:D:357:LEU:HD12	1:D:357:LEU:N	2.28	0.49
1:D:405:CYS:HB2	2:D:501:HEM:C1A	2.48	0.49
1:A:220:ASP:OD1	1:A:258:ARG:HD3	2.12	0.49
1:B:76:HIS:ND1	1:B:77:PRO:HD3	2.28	0.49
1:C:19:HIS:ND1	1:C:46:LEU:HA	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:TRP:CE2	1:C:142:VAL:HG11	2.47	0.49
1:A:398:PHE:CD2	1:A:408:ARG:HD2	2.48	0.49
1:D:208:TYR:O	1:D:211:ASP:HB2	2.13	0.49
1:B:106:ILE:HD13	1:B:252:LEU:HG	1.95	0.49
1:C:84:ASN:HD22	1:C:190:MET:HE1	1.77	0.49
1:D:174:HIS:CD2	1:D:176:PHE:HB3	2.47	0.49
1:A:431:PRO:HG3	1:A:452:ARG:HG3	1.95	0.48
1:B:135:GLU:O	1:B:138:GLN:HG3	2.12	0.48
1:C:81:ASN:HB3	1:C:190:MET:HE3	1.95	0.48
1:C:309:TYR:CE2	1:C:313:MET:HG3	2.48	0.48
1:C:332:ILE:HD12	2:C:501:HEM:C4A	2.48	0.48
1:A:76:HIS:CG	1:A:77:PRO:HD3	2.48	0.48
1:A:108:LEU:HB3	1:A:109:PRO:HD3	1.94	0.48
1:A:184:MET:SD	1:A:266:ILE:HG23	2.53	0.48
1:C:38:GLN:O	1:C:40:PRO:HD3	2.13	0.48
1:C:283:LEU:HD21	1:C:321:ILE:HD13	1.94	0.48
1:D:156:ILE:HD11	2:D:501:HEM:HBC1	1.94	0.48
1:D:432:TYR:HA	3:D:503:SO4:O1	2.14	0.48
1:C:297:VAL:HG22	1:C:420:LEU:HD12	1.95	0.48
1:A:85:LEU:CD1	1:A:266:ILE:CD1	2.63	0.48
1:B:268:GLY:O	1:B:270:GLU:N	2.46	0.48
1:D:116:MET:HA	1:D:119:TYR:HD2	1.78	0.48
1:A:176:PHE:HZ	1:A:262:MET:HE1	1.77	0.48
1:D:65:LEU:CD2	1:D:357:LEU:HB2	2.44	0.48
1:B:107:LEU:O	1:B:108:LEU:C	2.56	0.48
1:D:174:HIS:ND1	1:D:175:PRO:HD2	2.28	0.48
1:A:314:ARG:CG	1:A:314:ARG:O	2.62	0.48
1:D:176:PHE:CD2	1:D:215:MET:HA	2.49	0.48
1:B:107:LEU:CD1	1:B:264:PHE:HZ	2.25	0.47
1:A:361:ILE:CG2	1:A:365:HIS:CE1	2.97	0.47
1:B:188:MET:CE	1:B:442:LEU:HB2	2.40	0.47
1:B:287:PRO:HB3	1:C:287:PRO:HB3	1.96	0.47
1:B:328:PHE:CD2	1:B:366:ARG:NH2	2.82	0.47
1:D:464:VAL:HB	1:D:465:PRO:HD3	1.95	0.47
1:D:119:TYR:HE1	1:D:236:LEU:CD2	2.27	0.47
1:D:189:THR:C	1:D:191:PHE:H	2.23	0.47
1:D:218:LEU:C	1:D:218:LEU:HD23	2.40	0.47
1:D:332:ILE:HG13	1:D:443:THR:CG2	2.31	0.47
1:B:39:ILE:HG13	1:B:57:TYR:OH	2.14	0.47
1:B:33:PHE:HZ	1:B:366:ARG:HD2	1.75	0.47
1:B:91:PHE:HB2	1:B:263:THR:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:ARG:HG3	1:C:87:GLY:O	2.15	0.47
1:B:124:LEU:HD11	1:B:128:GLN:NE2	2.29	0.47
1:B:317:VAL:O	1:B:321:ILE:HG13	2.15	0.47
1:C:73:LYS:HE3	1:C:79:TYR:CE2	2.49	0.47
1:D:209:TRP:HA	1:D:212:ILE:CD1	2.41	0.47
1:B:23:LEU:HD11	1:B:48:ILE:HG22	1.97	0.46
1:B:221:GLU:OE1	1:B:224:ARG:NH1	2.47	0.46
1:C:19:HIS:ND1	1:C:46:LEU:HB2	2.30	0.46
1:D:371:TRP:HE1	1:D:394:ALA:HB1	1.80	0.46
1:A:227:ARG:NH1	1:A:254:ASP:OD1	2.48	0.46
1:B:283:LEU:HB3	1:B:290:LEU:HD13	1.98	0.46
1:C:138:GLN:OE1	1:C:454:ARG:HD3	2.15	0.46
1:C:439:LYS:O	1:C:444:ILE:HA	2.16	0.46
1:A:65:LEU:HD21	1:A:357:LEU:HB3	1.97	0.46
1:C:240:MET:HE1	1:C:257:ILE:HA	1.97	0.46
1:D:190:MET:HE1	1:D:208:TYR:CZ	2.49	0.46
1:C:239:LEU:C	1:C:239:LEU:HD23	2.41	0.46
1:C:316:ASP:OD2	1:C:320:ARG:NH1	2.48	0.46
2:A:501:HEM:HBB2	2:A:501:HEM:CMB	2.39	0.46
1:B:270:GLU:HG2	1:B:445:LYS:HE3	1.97	0.46
1:B:130:LEU:HD11	1:B:134:TRP:NE1	2.31	0.46
1:B:227:ARG:HH12	1:B:254:ASP:CG	2.23	0.46
1:C:14:HIS:ND1	1:C:15:PRO:HD2	2.31	0.46
1:C:36:ALA:HB1	1:C:57:TYR:CE2	2.51	0.46
1:A:383:THR:O	1:A:387:ARG:HB2	2.15	0.46
1:B:240:MET:HE1	1:B:260:GLN:CB	2.46	0.46
1:D:157:SER:OG	1:D:165:PHE:HE2	1.99	0.46
1:A:262:MET:HA	1:A:262:MET:HE2	1.97	0.46
1:C:22:TYR:CD1	1:C:35:LEU:HD11	2.51	0.45
1:D:409:GLN:H	1:D:409:GLN:CD	2.23	0.45
1:C:240:MET:CE	1:C:257:ILE:HG23	2.36	0.45
1:A:66:THR:O	1:A:66:THR:CG2	2.63	0.45
1:C:297:VAL:HG21	1:C:423:LEU:HB2	1.98	0.45
1:D:256:ASN:O	1:D:260:GLN:HG2	2.17	0.45
1:C:220:ASP:O	1:C:223:ILE:HB	2.17	0.45
1:A:76:HIS:CG	1:A:77:PRO:N	2.85	0.45
1:A:217:GLU:OE2	1:C:40:PRO:HD2	2.16	0.45
1:A:287:PRO:HD2	1:D:428:LEU:O	2.17	0.45
1:A:315:LEU:HD11	1:A:420:LEU:HD22	1.99	0.45
1:B:61:LEU:O	1:B:65:LEU:HG	2.16	0.45
1:C:11:PRO:HD3	1:C:45:GLN:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:PHE:CE2	1:C:309:TYR:HA	2.52	0.45
1:C:378:ASP:HB3	1:C:381:ARG:HG3	1.98	0.45
1:D:120:PHE:CE2	1:D:309:TYR:N	2.85	0.45
1:D:120:PHE:O	1:D:121:GLY:C	2.57	0.45
1:B:380:ASP:HB2	1:C:457:ARG:HH21	1.81	0.45
1:D:152:THR:CG2	1:D:272:THR:HG22	2.47	0.45
1:B:431:PRO:HD3	1:B:451:LEU:HA	1.99	0.45
1:C:106:ILE:O	1:C:109:PRO:HD2	2.17	0.45
1:C:309:TYR:CE2	1:C:313:MET:CG	2.99	0.45
1:D:103:ALA:CB	1:D:260:GLN:NE2	2.80	0.45
1:D:276:LEU:HD21	1:D:415:ALA:HA	1.98	0.45
1:B:58:ASP:HB3	1:B:61:LEU:CD1	2.47	0.45
1:D:245:ASP:HB3	1:D:249:GLY:H	1.82	0.45
1:A:122:GLN:HB3	1:A:158:LEU:HG	1.99	0.45
1:B:184:MET:HE3	1:B:184:MET:HB3	1.79	0.45
1:B:236:LEU:O	1:B:240:MET:HG3	2.17	0.45
1:D:120:PHE:CZ	1:D:308:THR:HA	2.50	0.45
2:D:501:HEM:HBC2	2:D:501:HEM:CMC	2.45	0.45
1:A:73:LYS:HE3	1:A:79:TYR:CE2	2.53	0.44
1:C:107:LEU:O	1:C:108:LEU:C	2.59	0.44
1:D:42:GLY:HA3	1:D:58:ASP:HB2	1.98	0.44
1:C:138:GLN:NE2	1:C:455:GLU:HG3	2.33	0.44
1:D:153:LEU:HD13	1:D:177:LEU:HD13	1.98	0.44
1:A:61:LEU:N	1:A:61:LEU:HD23	2.31	0.44
1:A:75:VAL:HG23	1:A:94:ASP:OD1	2.18	0.44
1:D:113:GLN:O	1:D:116:MET:HG2	2.18	0.44
1:B:130:LEU:HD12	1:B:130:LEU:C	2.42	0.44
1:D:49:GLN:C	1:D:51:ARG:H	2.26	0.44
1:A:82:ILE:HA	1:A:187:THR:HG21	2.00	0.44
1:A:412:LEU:HD23	1:A:412:LEU:HA	1.74	0.44
1:B:108:LEU:N	1:B:109:PRO:CD	2.81	0.44
1:B:161:PHE:CE1	1:B:163:TYR:HB3	2.51	0.44
1:C:240:MET:HB3	1:C:257:ILE:HG12	1.99	0.44
1:D:11:PRO:HB3	1:D:35:LEU:HD23	2.00	0.44
1:B:13:LYS:HG2	1:B:18:GLY:HA2	1.99	0.44
1:B:269:HIS:CG	1:B:270:GLU:N	2.85	0.44
1:C:428:LEU:HD23	1:C:453:VAL:HG12	2.00	0.44
1:B:278:PHE:CZ	1:B:446:PRO:HD3	2.53	0.44
1:B:308:THR:OG1	1:B:310:ASP:HB3	2.18	0.44
1:C:197:LEU:HD11	1:C:202:GLU:HB2	2.00	0.44
1:B:91:PHE:CB	1:B:263:THR:HG23	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:LEU:CD1	1:B:315:LEU:HD12	2.43	0.43
1:C:46:LEU:CD1	1:C:48:ILE:CG2	2.96	0.43
1:C:240:MET:HE3	1:C:257:ILE:HA	1.97	0.43
1:A:64:GLU:OE2	1:A:346:GLY:N	2.35	0.43
1:D:278:PHE:O	1:D:282:LEU:HG	2.18	0.43
1:D:329:TRP:O	1:D:330:SER:C	2.58	0.43
1:A:94:ASP:HB3	1:A:96:PHE:CE2	2.53	0.43
1:A:330:SER:OG	1:A:365:HIS:HE1	2.01	0.43
1:C:240:MET:HE2	1:C:257:ILE:CG2	2.35	0.43
1:D:161:PHE:CD2	1:D:161:PHE:O	2.71	0.43
1:D:245:ASP:HB3	1:D:248:THR:OG1	2.18	0.43
1:C:89:GLY:HA2	1:C:260:GLN:NE2	2.34	0.43
1:A:85:LEU:C	1:A:85:LEU:HD12	2.43	0.43
1:C:252:LEU:HD22	1:C:256:ASN:OD1	2.17	0.43
1:D:156:ILE:HD11	2:D:501:HEM:CBC	2.49	0.43
1:A:297:VAL:HG22	1:A:420:LEU:CD1	2.48	0.43
1:A:330:SER:OG	1:A:365:HIS:CE1	2.72	0.43
1:B:108:LEU:CB	1:B:109:PRO:HD3	2.48	0.43
1:C:68:GLU:HA	1:C:71:PHE:O	2.19	0.43
1:D:108:LEU:HD23	1:D:108:LEU:HA	1.76	0.43
1:A:284:LEU:HD23	1:A:284:LEU:HA	1.78	0.43
1:A:326:LEU:HD23	1:A:326:LEU:HA	1.78	0.43
1:A:357:LEU:N	1:A:357:LEU:HD22	2.33	0.43
1:B:197:LEU:HA	1:B:201:MET:HE3	2.00	0.43
1:B:300:LEU:HD12	1:B:315:LEU:CD1	2.46	0.43
1:C:65:LEU:HD21	1:C:357:LEU:HD22	2.01	0.43
1:D:431:PRO:HG3	1:D:452:ARG:HG2	1.99	0.43
1:B:75:VAL:HG21	1:B:93:SER:C	2.44	0.43
1:C:122:GLN:H	1:C:122:GLN:NE2	2.17	0.43
1:D:82:ILE:HG23	1:D:92:THR:CG2	2.47	0.43
1:D:152:THR:HG21	1:D:272:THR:HG22	2.01	0.43
1:C:124:LEU:HD12	1:C:124:LEU:O	2.18	0.42
1:B:153:LEU:HG	1:B:269:HIS:CD2	2.53	0.42
1:C:71:PHE:HD2	1:C:339:ALA:HA	1.84	0.42
1:D:81:ASN:O	1:D:84:ASN:HB2	2.19	0.42
1:D:378:ASP:O	1:D:381:ARG:HG3	2.18	0.42
1:A:135:GLU:O	1:A:138:GLN:HG3	2.19	0.42
1:B:221:GLU:O	1:B:225:GLU:HG2	2.19	0.42
1:D:12:PRO:HG2	1:D:22:TYR:OH	2.19	0.42
1:A:297:VAL:HG22	1:A:420:LEU:HD12	2.01	0.42
1:C:245:ASP:O	1:C:247:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:ALA:HB1	1:B:57:TYR:CE2	2.55	0.42
1:B:280:LEU:HD23	1:B:280:LEU:HA	1.84	0.42
1:C:290:LEU:HD12	1:C:290:LEU:O	2.19	0.42
1:A:126:VAL:HG12	1:A:151:LEU:HD12	2.02	0.42
1:C:338:THR:HG22	1:C:339:ALA:N	2.35	0.42
1:D:176:PHE:HD2	1:D:215:MET:HA	1.84	0.42
1:A:153:LEU:CD1	1:A:269:HIS:CG	3.02	0.42
1:A:193:ARG:HD2	1:A:193:ARG:HA	1.90	0.42
1:D:405:CYS:HA	2:D:501:HEM:CHA	2.50	0.42
1:A:152:THR:HG22	1:A:414:GLU:OE1	2.20	0.42
1:A:275:LEU:HD21	1:A:322:LEU:HD22	2.02	0.42
1:B:58:ASP:O	1:B:62:VAL:HG23	2.20	0.42
1:C:327:ARG:NH2	1:C:381:ARG:NH1	2.68	0.42
1:B:33:PHE:CE1	1:B:366:ARG:HD2	2.55	0.42
1:B:65:LEU:HA	1:B:71:PHE:CD1	2.55	0.42
1:B:75:VAL:HG21	1:B:92:THR:O	2.20	0.42
1:B:180:LEU:O	1:B:184:MET:HG2	2.19	0.42
1:D:216:ASN:HA	1:D:258:ARG:HD2	2.01	0.42
1:C:240:MET:CE	1:C:260:GLN:HB2	2.48	0.42
1:D:23:LEU:HD11	1:D:48:ILE:CG2	2.45	0.42
1:D:219:VAL:HG11	1:D:258:ARG:HG3	2.00	0.42
1:D:419:LEU:HD23	1:D:419:LEU:HA	1.86	0.42
1:A:10:SER:HA	1:A:11:PRO:HD3	1.92	0.41
1:A:165:PHE:O	1:A:166:ARG:C	2.63	0.41
1:A:367:HIS:ND1	1:A:369:ALA:HB3	2.35	0.41
1:A:398:PHE:HB3	1:A:405:CYS:HB3	2.00	0.41
1:A:457:ARG:HB2	1:A:460:GLU:HG3	2.01	0.41
1:C:161:PHE:CE1	1:C:163:TYR:CB	3.02	0.41
1:C:161:PHE:HD2	1:C:261:VAL:HG13	1.83	0.41
1:C:340:LEU:O	1:C:353:LYS:HG3	2.20	0.41
1:C:405:CYS:SG	1:C:408:ARG:N	2.93	0.41
1:D:245:ASP:OD1	1:D:248:THR:HG23	2.21	0.41
1:A:405:CYS:HB2	2:A:501:HEM:C4A	2.56	0.41
1:B:107:LEU:HD13	1:B:264:PHE:CZ	2.48	0.41
1:C:46:LEU:CD1	1:C:48:ILE:HG23	2.49	0.41
1:D:241:LEU:HD23	1:D:257:ILE:HD13	2.02	0.41
1:A:55:GLN:HE22	1:A:334:ASN:HD21	1.67	0.41
1:B:284:LEU:HD23	1:B:284:LEU:HA	1.42	0.41
1:C:84:ASN:ND2	1:C:190:MET:HE1	2.34	0.41
1:C:285:ARG:HA	1:C:285:ARG:HD3	1.65	0.41
1:C:421:LEU:HA	1:C:421:LEU:HD23	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:409:GLN:CD	1:D:409:GLN:N	2.78	0.41
1:B:37:ARG:HD3	1:B:37:ARG:HA	1.77	0.41
1:B:124:LEU:O	1:B:128:GLN:HG3	2.20	0.41
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	2.03	0.41
1:C:332:ILE:O	1:C:332:ILE:HG22	2.21	0.41
1:D:149:THR:HG23	1:D:269:HIS:NE2	2.35	0.41
1:A:398:PHE:CE2	1:A:408:ARG:HG3	2.55	0.41
1:C:11:PRO:HG3	1:C:44:PHE:CD1	2.56	0.41
1:A:72:GLN:HG3	1:A:340:LEU:HD11	2.02	0.41
1:A:241:LEU:HD23	1:A:241:LEU:HA	1.81	0.41
1:C:284:LEU:HD23	1:C:284:LEU:HA	1.92	0.41
1:D:108:LEU:HA	1:D:406:ILE:HD11	2.02	0.41
1:D:120:PHE:HZ	1:D:307:PRO:O	2.04	0.41
1:D:125:GLU:OE1	1:D:164:ARG:NH1	2.54	0.41
1:D:255:GLU:O	1:D:259:TYR:CD1	2.70	0.41
1:A:161:PHE:CD1	1:A:161:PHE:N	2.88	0.41
1:B:41:GLU:OE1	1:B:41:GLU:N	2.45	0.41
1:B:120:PHE:CE2	1:B:308:THR:HA	2.55	0.41
1:B:403:ARG:HA	1:B:403:ARG:HD2	1.81	0.41
1:C:218:LEU:C	1:C:218:LEU:HD23	2.46	0.41
1:D:83:ARG:HA	1:D:92:THR:HG21	2.01	0.41
1:D:308:THR:O	1:D:311:THR:HB	2.21	0.41
1:D:312:VAL:HA	1:D:315:LEU:HD12	2.03	0.41
1:C:37:ARG:HH21	1:C:366:ARG:CB	2.34	0.41
1:C:134:TRP:CZ2	1:C:142:VAL:HG11	2.55	0.41
1:C:257:ILE:O	1:C:261:VAL:HG23	2.21	0.41
1:C:310:ASP:O	1:C:311:THR:C	2.63	0.41
1:C:396:LYS:NZ	1:C:400:ASN:OD1	2.50	0.41
1:A:153:LEU:HD13	1:A:269:HIS:CG	2.56	0.41
1:B:37:ARG:NH2	1:B:366:ARG:C	2.79	0.41
1:B:152:THR:O	1:B:156:ILE:HG22	2.21	0.41
1:B:258:ARG:O	1:B:262:MET:HG2	2.21	0.41
1:B:278:PHE:CE2	1:B:446:PRO:HD3	2.56	0.41
1:B:287:PRO:HB2	1:C:290:LEU:HD23	2.03	0.41
1:C:48:ILE:O	1:C:50:GLY:N	2.54	0.41
1:C:102:LYS:O	1:C:106:ILE:HG13	2.20	0.41
1:C:126:VAL:HG12	1:C:151:LEU:CD1	2.46	0.41
1:D:361:ILE:HA	1:D:361:ILE:HD13	1.86	0.41
1:A:287:PRO:HB3	1:D:287:PRO:HB3	2.02	0.41
1:A:120:PHE:CE1	1:A:124:LEU:HD22	2.56	0.40
1:A:149:THR:O	1:A:153:LEU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:GLY:O	1:A:408:ARG:C	2.63	0.40
1:B:173:LEU:HA	1:B:173:LEU:HD23	1.76	0.40
1:D:79:TYR:HA	1:D:82:ILE:HG22	2.03	0.40
1:D:156:ILE:HG21	1:D:265:LEU:HD23	2.03	0.40
1:A:42:GLY:CA	1:A:58:ASP:HB2	2.51	0.40
1:A:59:PRO:HB3	1:A:391:HIS:CD2	2.57	0.40
1:A:366:ARG:NH1	1:A:375:ASP:OD1	2.53	0.40
1:A:391:HIS:ND1	1:A:392:PRO:HD2	2.36	0.40
1:B:39:ILE:CD1	1:B:44:PHE:HB3	2.51	0.40
1:C:79:TYR:CD1	1:C:79:TYR:N	2.90	0.40
1:C:144:VAL:O	1:C:145:ALA:C	2.62	0.40
1:C:240:MET:HE2	1:C:257:ILE:HG12	2.03	0.40
1:C:412:LEU:HD23	1:C:412:LEU:HA	1.94	0.40
1:D:64:GLU:HG2	1:D:70:ARG:HH12	1.86	0.40
1:B:315:LEU:HB3	1:B:319:PRO:HD3	2.03	0.40
1:A:176:PHE:CZ	1:A:262:MET:HE1	2.55	0.40
1:B:39:ILE:CG1	1:B:57:TYR:OH	2.70	0.40
1:C:160:GLY:HA2	1:C:236:LEU:HD12	2.03	0.40
1:D:126:VAL:HG12	1:D:151:LEU:HD12	2.02	0.40
1:D:317:VAL:O	1:D:321:ILE:HG13	2.21	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	462/493 (94%)	439 (95%)	21 (4%)	2 (0%)	30	48
1	B	458/493 (93%)	435 (95%)	16 (4%)	7 (2%)	8	18
1	C	451/493 (92%)	420 (93%)	26 (6%)	5 (1%)	11	24
1	D	434/493 (88%)	399 (92%)	31 (7%)	4 (1%)	14	28
All	All	1805/1972 (92%)	1693 (94%)	94 (5%)	18 (1%)	12	25

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	PRO
1	B	77	PRO
1	B	235	ASP
1	C	77	PRO
1	D	77	PRO
1	B	51	ARG
1	B	230	GLY
1	D	78	ALA
1	A	76	HIS
1	B	249	GLY
1	B	269	HIS
1	C	49	GLN
1	C	76	HIS
1	C	249	GLY
1	C	441	SER
1	D	15	PRO
1	D	190	MET
1	B	76	HIS

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	392/416 (94%)	378 (96%)	14 (4%)	31	56
1	B	388/416 (93%)	376 (97%)	12 (3%)	35	60
1	C	388/416 (93%)	372 (96%)	16 (4%)	27	52
1	D	374/416 (90%)	361 (96%)	13 (4%)	32	57
All	All	1542/1664 (93%)	1487 (96%)	55 (4%)	31	56

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	61	LEU

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Mol	Chain	Res	Type
1	A	122	GLN
1	A	149	THR
1	A	184	MET
1	A	198	THR
1	A	263	THR
1	A	299	ARG
1	A	344	VAL
1	A	345	ILE
1	A	357	LEU
1	A	372	THR
1	A	383	THR
1	A	425	LYS
1	B	5	LEU
1	B	39	ILE
1	B	92	THR
1	B	154	ASP
1	B	190	MET
1	B	203	GLU
1	B	221	GLU
1	B	251	ARG
1	B	270	GLU
1	B	344	VAL
1	B	366	ARG
1	B	403	ARG
1	C	16	GLN
1	C	51	ARG
1	C	66	THR
1	C	122	GLN
1	C	171	ASP
1	C	182	ARG
1	C	190	MET
1	C	221	GLU
1	C	251	ARG
1	C	269	HIS
1	C	299	ARG
1	C	328	PHE
1	C	389	THR
1	C	422	ILE
1	C	438	VAL
1	C	447	GLU
1	D	5	LEU
1	D	15	PRO

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Mol	Chain	Res	Type
1	D	52	THR
1	D	77	PRO
1	D	92	THR
1	D	156	ILE
1	D	269	HIS
1	D	284	LEU
1	D	304	ASP
1	D	348	LYS
1	D	351	ILE
1	D	389	THR
1	D	402	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	334	ASN
1	A	365	HIS
1	A	386	ASN
1	B	81	ASN
1	B	99	ASN
1	B	269	HIS
1	B	334	ASN
1	C	122	GLN
1	C	140	GLN
1	C	334	ASN
1	D	14	HIS
1	D	55	GLN
1	D	76	HIS
1	D	81	ASN
1	D	174	HIS
1	D	334	ASN
1	D	341	GLN
1	D	365	HIS
1	D	409	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 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	C	501	-	50,50,50	1.42	10 (20%)	67,82,82	1.18	6 (8%)
3	SO4	D	503	-	4,4,4	0.41	0	6,6,6	0.50	0
3	SO4	C	502	-	4,4,4	0.33	0	6,6,6	0.37	0
3	SO4	D	502	-	4,4,4	0.28	0	6,6,6	0.53	0
3	SO4	A	502	-	4,4,4	0.23	0	6,6,6	0.54	0
2	HEM	A	501	1	50,50,50	1.47	11 (22%)	67,82,82	1.26	5 (7%)
2	HEM	D	501	1	50,50,50	1.59	9 (18%)	67,82,82	1.11	4 (5%)
3	SO4	B	503	-	4,4,4	0.22	0	6,6,6	0.46	0
3	SO4	C	504	-	4,4,4	0.31	0	6,6,6	0.37	0
3	SO4	B	504	-	4,4,4	0.43	0	6,6,6	0.09	0
3	SO4	C	503	-	4,4,4	0.18	0	6,6,6	0.30	0
2	HEM	B	501	-	50,50,50	1.45	10 (20%)	67,82,82	1.29	8 (11%)
3	SO4	B	502	-	4,4,4	0.31	0	6,6,6	0.12	0
3	SO4	A	503	-	4,4,4	0.36	0	6,6,6	0.58	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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	501	1	-	2/14/54/54	-
2	HEM	D	501	1	-	2/14/54/54	-
2	HEM	C	501	-	-	2/14/54/54	-
2	HEM	B	501	-	-	3/14/54/54	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	FE-ND	4.29	2.08	1.94
2	D	501	HEM	FE-NA	4.24	2.09	1.95
2	C	501	HEM	FE-NC	4.02	2.08	1.95
2	D	501	HEM	FE-NB	3.79	2.06	1.94
2	A	501	HEM	FE-NC	3.30	2.06	1.95
2	B	501	HEM	FE-ND	3.29	2.05	1.94
2	A	501	HEM	FE-NA	3.15	2.05	1.95
2	B	501	HEM	O1D-CGD	3.05	1.32	1.22
2	D	501	HEM	CAB-C3B	3.04	1.55	1.47
2	C	501	HEM	CAB-C3B	3.01	1.55	1.47
2	A	501	HEM	FE-ND	2.99	2.04	1.94
2	B	501	HEM	FE-NC	2.94	2.04	1.95
2	A	501	HEM	CAB-C3B	2.91	1.55	1.47
2	B	501	HEM	CMA-C3A	2.89	1.56	1.50
2	A	501	HEM	CAC-C3C	2.82	1.54	1.47
2	D	501	HEM	CAC-C3C	2.78	1.54	1.47
2	C	501	HEM	FE-NB	2.73	2.03	1.94
2	B	501	HEM	CMB-C2B	2.65	1.56	1.50
2	A	501	HEM	CMC-C2C	2.64	1.56	1.50
2	B	501	HEM	O1A-CGA	2.56	1.30	1.22
2	D	501	HEM	CMA-C3A	2.46	1.55	1.50
2	A	501	HEM	CMB-C2B	2.44	1.55	1.50
2	D	501	HEM	CMD-C2D	2.39	1.55	1.50
2	A	501	HEM	CMD-C2D	2.38	1.55	1.50
2	C	501	HEM	CAC-C3C	2.38	1.53	1.47
2	A	501	HEM	CAD-C3D	2.36	1.57	1.51
2	B	501	HEM	CMD-C2D	2.34	1.55	1.50
2	C	501	HEM	CMB-C2B	2.32	1.55	1.50
2	B	501	HEM	CAC-C3C	2.32	1.53	1.47
2	A	501	HEM	CMA-C3A	2.30	1.55	1.50
2	B	501	HEM	CAB-C3B	2.25	1.53	1.47
2	D	501	HEM	CMC-C2C	2.25	1.55	1.50
2	C	501	HEM	CAA-C2A	2.24	1.57	1.51
2	B	501	HEM	CMC-C2C	2.22	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	CMB-C2B	2.21	1.55	1.50
2	C	501	HEM	C2A-C3A	-2.15	1.33	1.38
2	C	501	HEM	CMD-C2D	2.14	1.55	1.50
2	A	501	HEM	C2A-C3A	-2.04	1.33	1.38
2	C	501	HEM	C3C-C2C	-2.03	1.33	1.37
2	C	501	HEM	CMC-C2C	2.01	1.54	1.50

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CHC-C4B-NB	3.82	128.54	124.42
2	C	501	HEM	CHD-C1D-ND	3.60	128.30	124.42
2	B	501	HEM	CHC-C4B-NB	3.44	128.12	124.42
2	B	501	HEM	CAA-CBA-CGA	-3.18	105.23	113.67
2	A	501	HEM	CHD-C1D-ND	3.04	127.70	124.42
2	C	501	HEM	O1A-CGA-CBA	-2.73	114.42	123.09
2	C	501	HEM	CHC-C4B-NB	2.62	127.24	124.42
2	B	501	HEM	CHD-C4C-NC	2.56	127.24	124.45
2	B	501	HEM	CBB-CAB-C3B	-2.37	115.68	127.53
2	A	501	HEM	O1D-CGD-CBD	-2.35	115.63	123.09
2	D	501	HEM	C1B-NB-C4B	2.33	107.97	105.21
2	B	501	HEM	C3B-C4B-NB	-2.31	107.81	109.47
2	D	501	HEM	C3B-C4B-NB	-2.30	107.82	109.47
2	D	501	HEM	O1A-CGA-CBA	-2.25	115.96	123.09
2	B	501	HEM	C4C-C3C-C2C	2.20	108.72	106.81
2	A	501	HEM	C2A-C1A-NA	-2.20	107.71	110.15
2	D	501	HEM	C4A-C3A-C2A	2.17	109.31	106.82
2	C	501	HEM	C4A-C3A-C2A	2.17	109.30	106.82
2	C	501	HEM	O2A-CGA-CBA	2.13	120.73	114.00
2	B	501	HEM	C1B-NB-C4B	2.11	107.71	105.21
2	A	501	HEM	CHB-C1B-NB	2.07	126.93	124.37
2	B	501	HEM	CHD-C1D-ND	2.07	126.65	124.42
2	C	501	HEM	C4C-C3C-C2C	2.03	108.58	106.81

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	HEM	CAD-CBD-CGD-O1D
2	B	501	HEM	CAD-CBD-CGD-O2D
2	D	501	HEM	CAD-CBD-CGD-O2D
2	C	501	HEM	CAD-CBD-CGD-O2D

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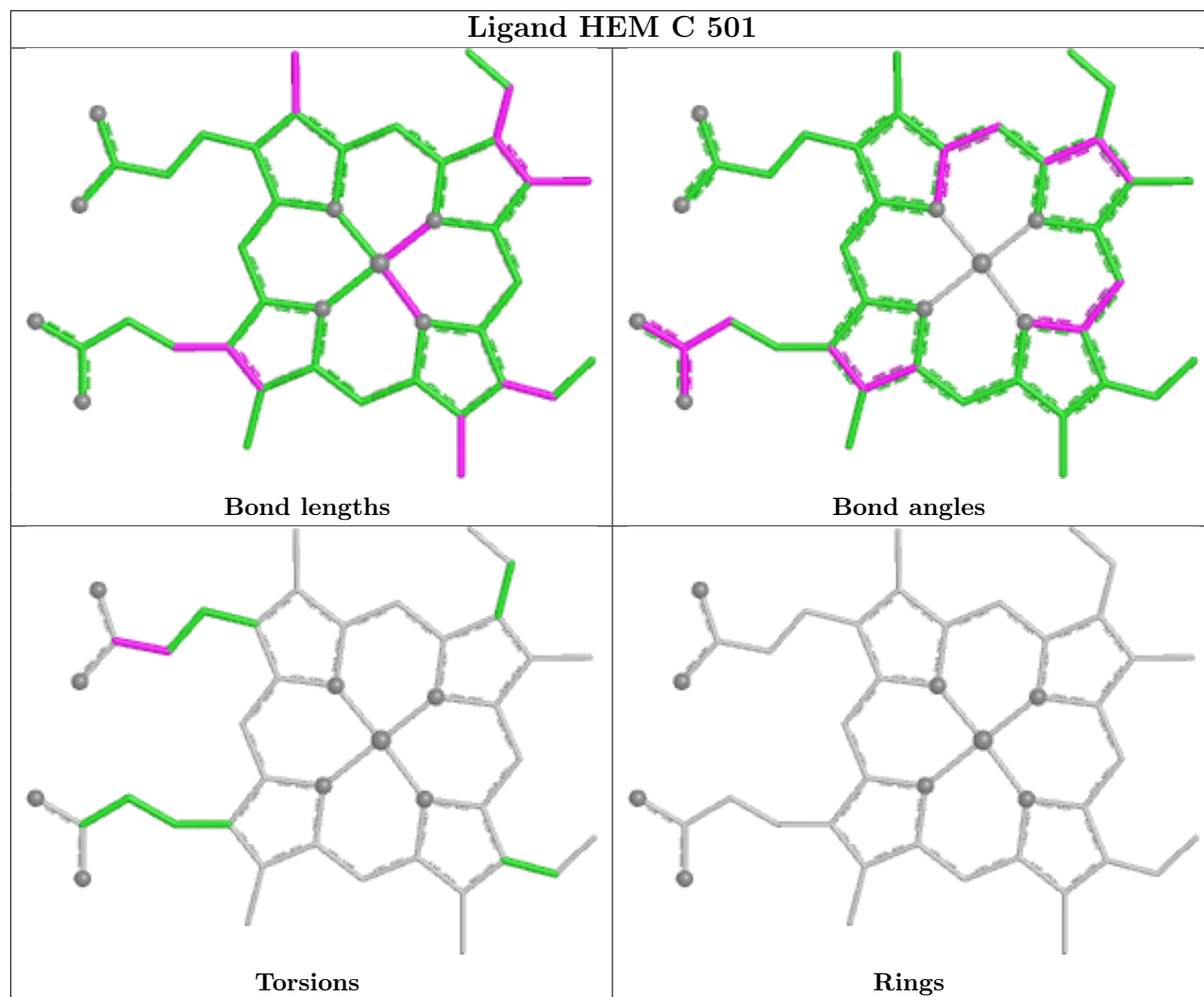
Mol	Chain	Res	Type	Atoms
2	D	501	HEM	CAD-CBD-CGD-O1D
2	C	501	HEM	CAD-CBD-CGD-O1D
2	A	501	HEM	CAD-CBD-CGD-O2D
2	A	501	HEM	CAD-CBD-CGD-O1D
2	B	501	HEM	CAA-CBA-CGA-O2A

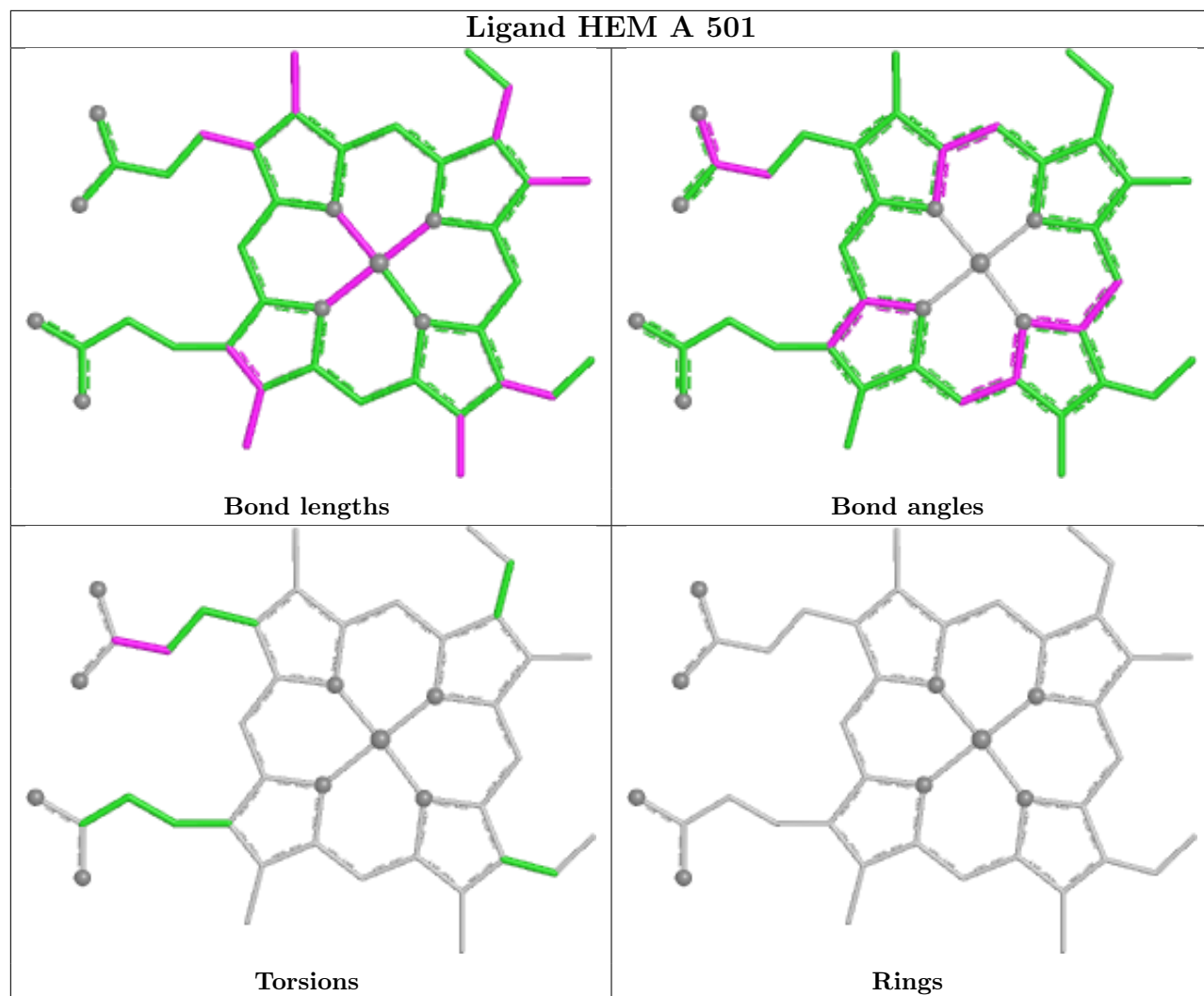
There are no ring outliers.

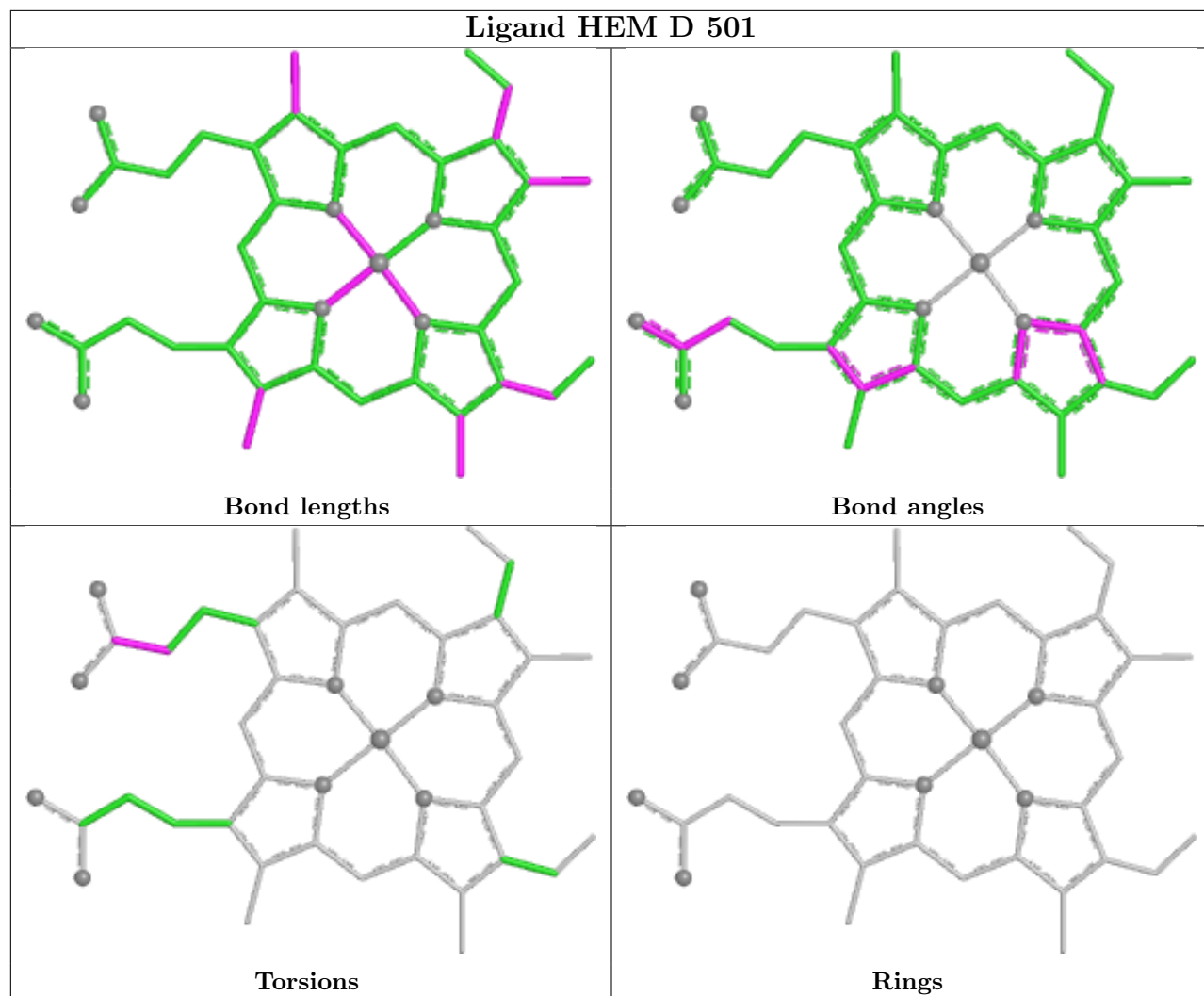
6 monomers are involved in 28 short contacts:

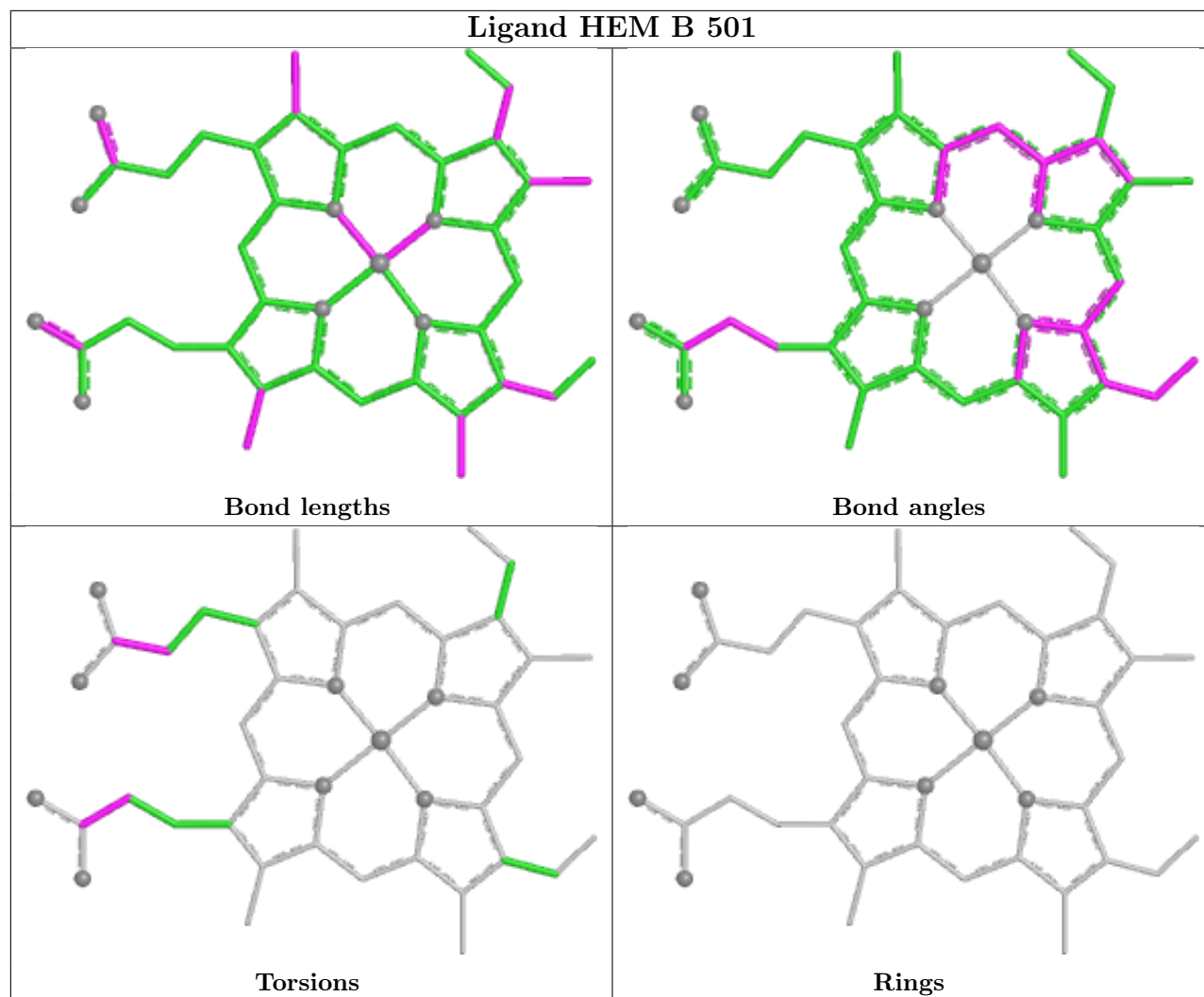
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	HEM	6	0
3	D	503	SO4	1	0
2	A	501	HEM	5	0
2	D	501	HEM	10	0
2	B	501	HEM	5	0
3	A	503	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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	464/493 (94%)	-0.19	22 (4%) 36 28	17, 33, 87, 131	0
1	B	460/493 (93%)	-0.13	13 (2%) 55 46	23, 43, 86, 127	0
1	C	454/493 (92%)	-0.32	9 (1%) 65 57	18, 36, 72, 118	1 (0%)
1	D	440/493 (89%)	0.13	20 (4%) 38 29	23, 46, 96, 120	0
All	All	1818/1972 (92%)	-0.13	64 (3%) 47 37	17, 40, 91, 131	1 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	183	ALA	4.8
1	D	465	PRO	4.0
1	B	264	PHE	3.9
1	A	15	PRO	3.8
1	B	234	GLY	3.7
1	A	197	LEU	3.4
1	B	235	ASP	3.3
1	D	247	GLU	3.3
1	B	464	VAL	3.2
1	B	197	LEU	3.1
1	A	13	LYS	3.1
1	B	5	LEU	3.0
1	D	462	PHE	3.0
1	D	243	ALA	2.9
1	C	387[A]	ARG	2.9
1	C	234	GLY	2.9
1	B	194	PRO	2.9
1	D	464	VAL	2.9
1	D	77	PRO	2.8
1	B	195	PRO	2.8
1	A	51	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	441	SER	2.7
1	B	233	GLY	2.7
1	B	196	VAL	2.7
1	A	14	HIS	2.7
1	A	196	VAL	2.7
1	A	53	LEU	2.7
1	A	4	ILE	2.6
1	A	12	PRO	2.6
1	C	197	LEU	2.6
1	A	191	PHE	2.6
1	C	192	SER	2.5
1	A	50	GLY	2.5
1	C	464	VAL	2.5
1	A	10	SER	2.5
1	A	447	GLU	2.5
1	A	9	PRO	2.5
1	B	193	ARG	2.5
1	D	443	THR	2.5
1	C	198	THR	2.4
1	C	225	GLU	2.4
1	D	203	GLU	2.4
1	D	88	ASP	2.4
1	D	184	MET	2.4
1	D	209	TRP	2.4
1	B	199	PRO	2.4
1	A	233	GLY	2.3
1	D	192	SER	2.3
1	A	18	GLY	2.3
1	D	4	ILE	2.3
1	D	442	LEU	2.2
1	A	19	HIS	2.2
1	A	47	ASP	2.2
1	C	201	MET	2.2
1	B	48	ILE	2.1
1	D	463	SER	2.1
1	A	245	ASP	2.1
1	C	304	ASP	2.1
1	A	247	GLU	2.1
1	D	78	ALA	2.1
1	A	232	GLY	2.0
1	D	82	ILE	2.0
1	A	194	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	238	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](#)

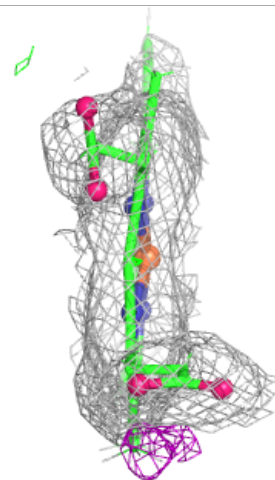
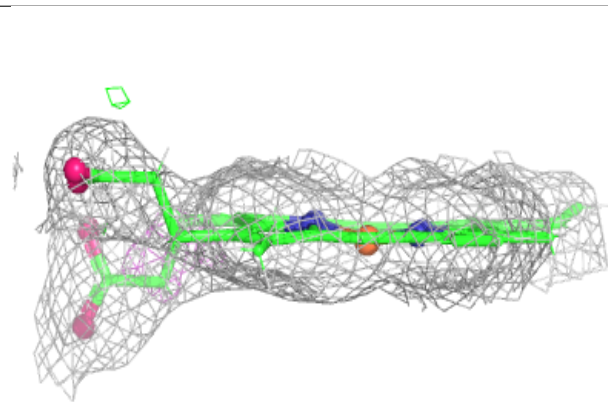
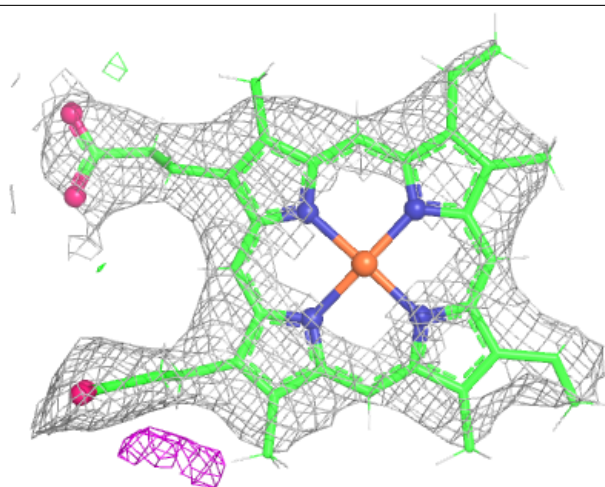
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	C	504	5/5	0.74	0.20	77,79,112,123	0
3	SO4	B	504	5/5	0.85	0.14	75,78,96,119	0
3	SO4	B	502	5/5	0.85	0.14	44,52,68,76	0
3	SO4	D	503	5/5	0.85	0.18	50,54,74,89	0
3	SO4	B	503	5/5	0.87	0.17	48,56,77,81	0
3	SO4	A	503	5/5	0.87	0.19	43,46,74,77	0
3	SO4	A	502	5/5	0.89	0.22	48,53,56,77	0
3	SO4	C	503	5/5	0.91	0.13	60,60,66,85	0
3	SO4	D	502	5/5	0.94	0.09	27,34,52,52	0
2	HEM	D	501	43/43	0.96	0.08	33,49,60,67	0
2	HEM	B	501	43/43	0.96	0.08	27,38,52,62	0
2	HEM	C	501	43/43	0.97	0.08	16,26,37,44	0
3	SO4	C	502	5/5	0.97	0.07	35,35,45,45	0
2	HEM	A	501	43/43	0.98	0.06	16,22,28,31	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.

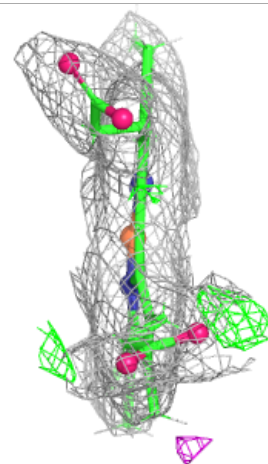
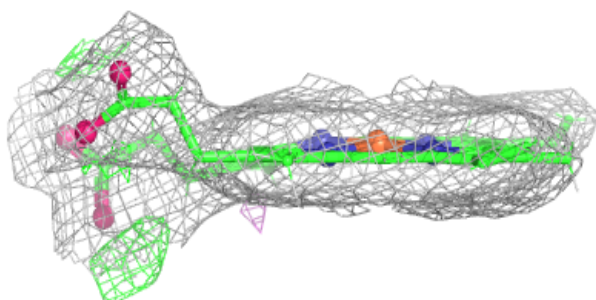
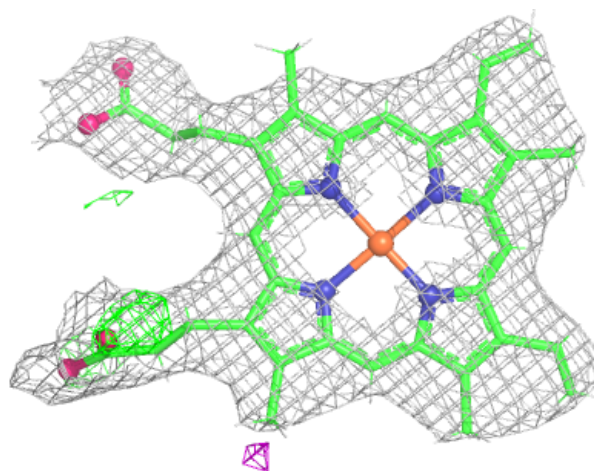
Electron density around HEM D 501:

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



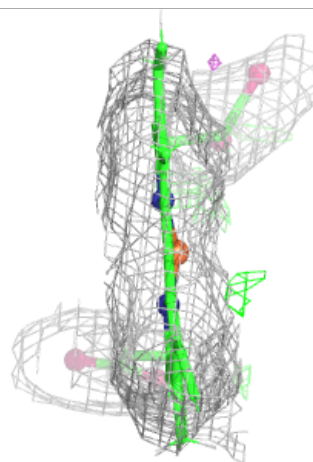
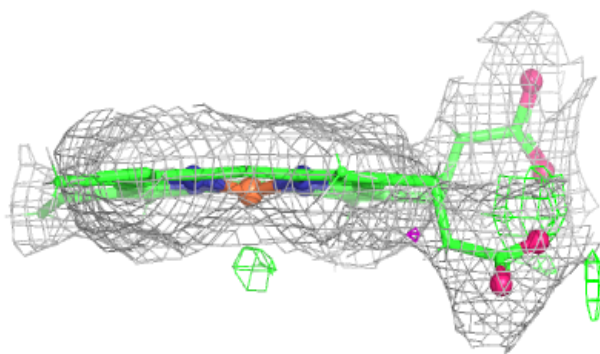
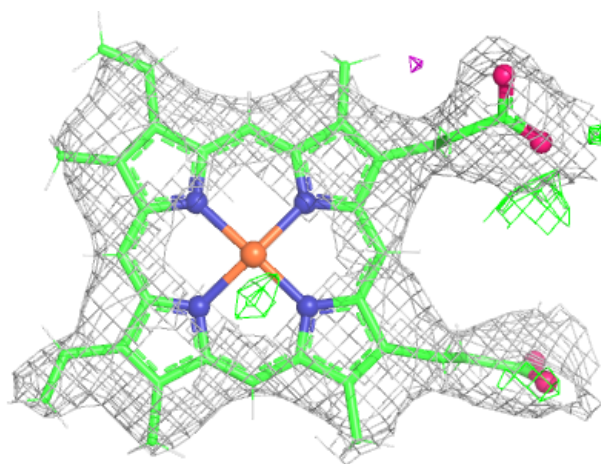
Electron density around HEM B 501:

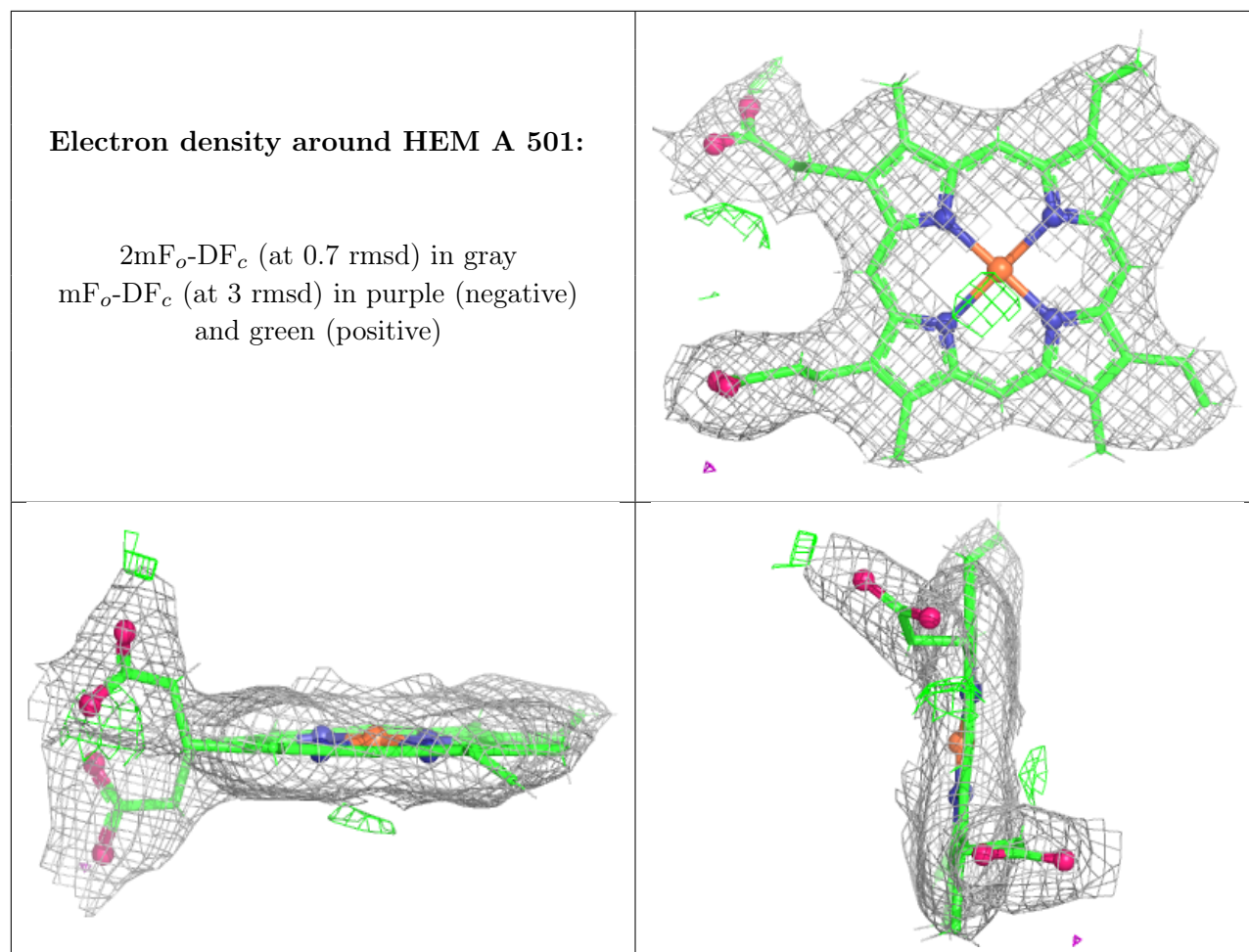
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.