



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2026 – 10:12 am BST

PDB ID : 9U2X / pdb_00009u2x
Title : Crystal structure of N244L variant from Bacillus subtilis
Authors : Borges, P.T.; Martins, L.O.
Deposited on : 2026-01-30
Resolution : 2.67 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 : 1.8.4, 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 : 9.0.010 (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

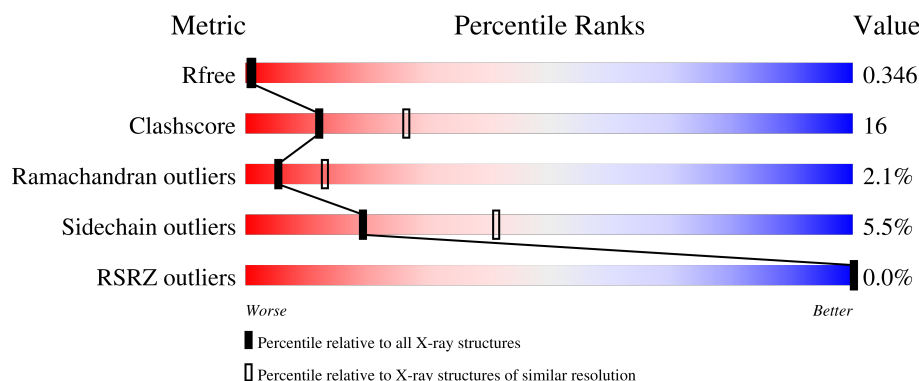
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.67 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	359	 65% 31% ..
1	B	359	 67% 29% ..
1	C	359	 65% 31% ..
1	D	359	 66% 29% ..
1	E	359	 66% 28% 5% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	359	<div><div></div><div>59%</div><div>35%</div><div></div><div>• •</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16847 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 Deferrochelataase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	0	0
			2754	1743	474	524	13			
1	B	354	Total	C	N	O	S	0	0	0
			2754	1743	474	524	13			
1	C	354	Total	C	N	O	S	0	0	0
			2754	1743	474	524	13			
1	D	353	Total	C	N	O	S	0	0	0
			2743	1737	470	523	13			
1	E	354	Total	C	N	O	S	0	0	0
			2754	1743	474	524	13			
1	F	354	Total	C	N	O	S	0	0	0
			2754	1743	474	524	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	244	LEU	ASN	variant	UNP P39597
B	244	LEU	ASN	variant	UNP P39597
C	244	LEU	ASN	variant	UNP P39597
D	244	LEU	ASN	variant	UNP P39597
E	244	LEU	ASN	variant	UNP P39597
F	244	LEU	ASN	variant	UNP P39597

- 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 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
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

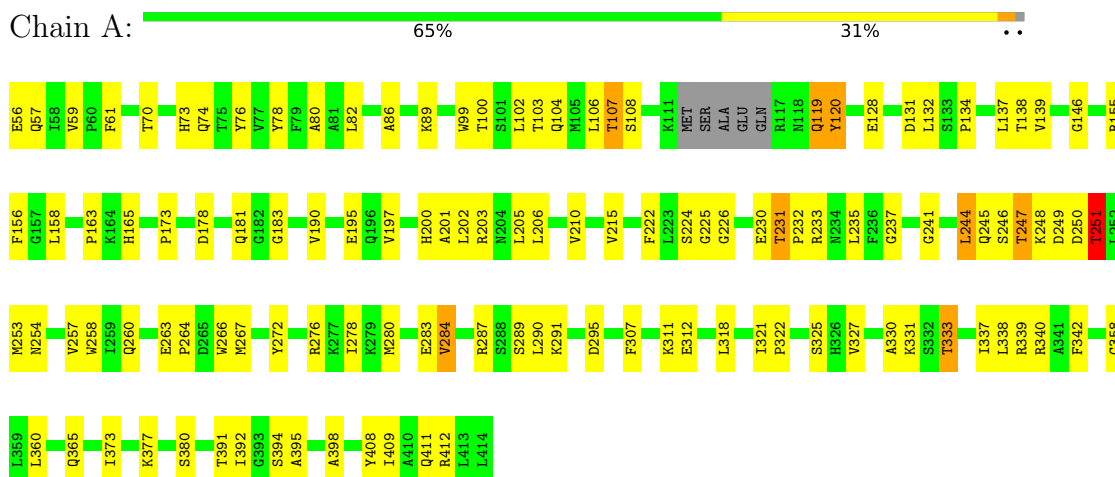
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	7	Total O 7 7	0	0
3	B	9	Total O 9 9	0	0
3	C	15	Total O 15 15	0	0
3	D	12	Total O 12 12	0	0
3	E	13	Total O 13 13	0	0
3	F	20	Total O 20 20	0	0

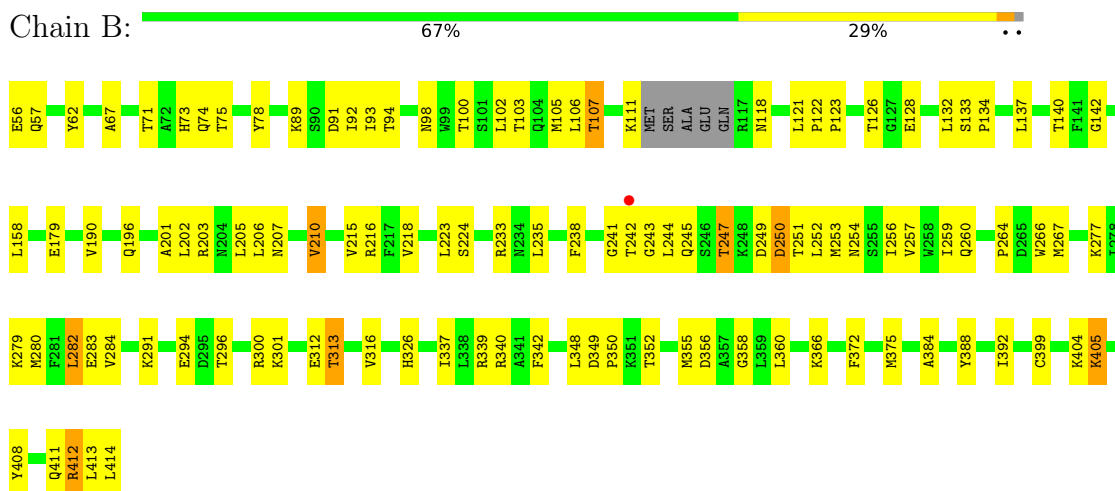
3 Residue-property plots

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: Deferrochelatase

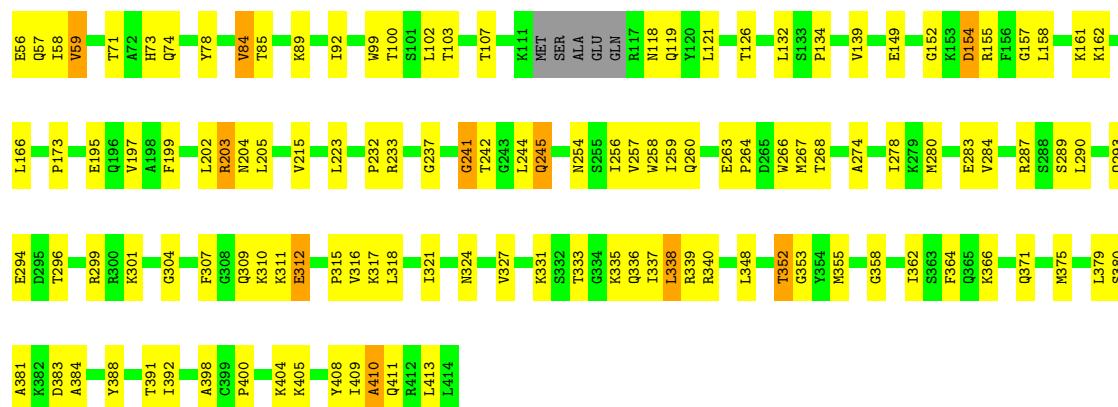


• Molecule 1: Deferrochelatase



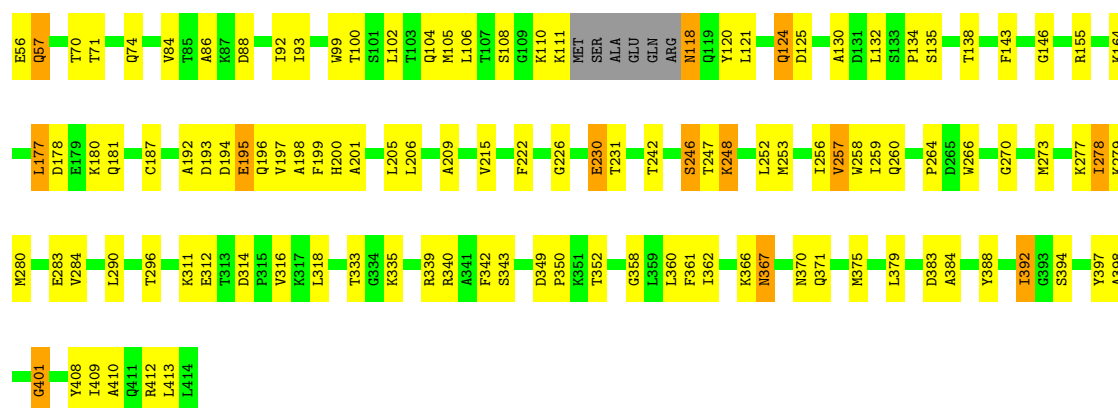
• Molecule 1: Deferrochelatase





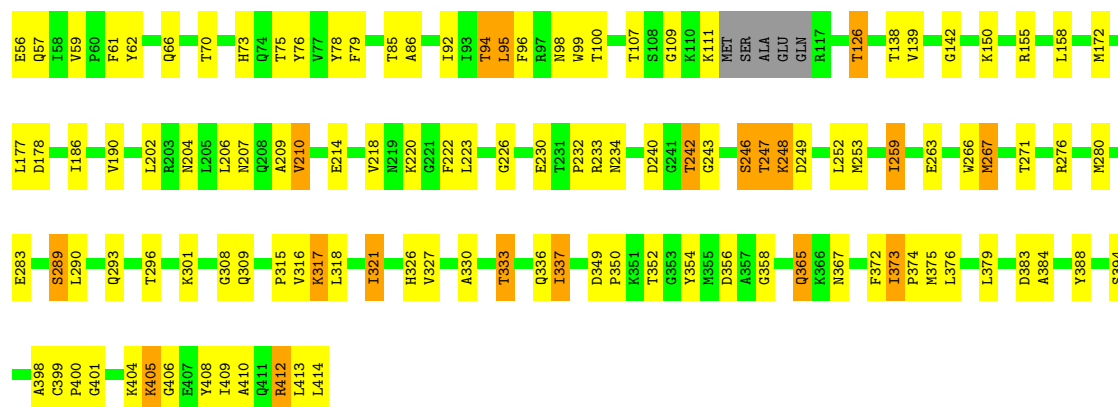
• Molecule 1: Deferrochelataase

Chain D: 66% 29% . .



• Molecule 1: Deferrochelataase

Chain E: 66% 28% 5% . .



• Molecule 1: Deferrochelataase

Chain F: 59% 35% . .

E56	Q57	I58	V59	P60	F61	H65	Q66	A67	H73	Q74	T75	Y76	V77	Y78	A81	L82	D83	V84	T85	A86	K87	D88	K89	I92	F96	W99	T100	T107	S108	K111	MET	SER	ALA	GLU	GLN	R117	P122	P123	T126	G127	E128	L132	S133	N136	V139			
G144	P145	G146	E149	Q150	F151	R155	K159	M172	L177	D178	E179	K180	Q181	G182	G183	G184	D185	I186	C187	V190	G191	A192	D193	D194	E195	Q196	V197	F199	H200	A201	L202	R203	N204	L205	L206	N207	Q208	A209	E214	V215	R216	F217	L223	K227	P232	R233	G237	F238
G241	L244	Q245	S246	M253	I259	E263	P264	D265	W266	M267	T268	G269	R276	K277	I278	K279	M280	V284	W285	D286	R287	S288	S289	L290	K291	D292	Q293	T296	R299	R300	K301	P306	F307	K311	V316	K317	L318	I321	P322	S323	N324	S325	H326	V327	S328	L329		
A330	K331	S332	T333	R339	R340	A341	T345	P350	L359	L360	F361	I362	Q365	K366	Q371	F372	M375	L376	K377	A378	L379	S380	A381	K382	D383	A384	Y388	T391	A395	A398	C399	P400	K404	K405	Y408	I409	R412	L413	L414									

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	351.93Å 73.88Å 127.23Å 90.00° 110.74° 90.00°	Depositor
Resolution (Å)	83.41 – 2.67 83.41 – 2.67	Depositor EDS
% Data completeness (in resolution range)	47.6 (83.41-2.67) 47.7 (83.41-2.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.297 , 0.348 0.298 , 0.346	Depositor DCC
R_{free} test set	2060 reflections (2.35%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.033 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16847	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: 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	0.15	0/2813	0.45	0/3791
1	B	0.15	0/2813	0.45	0/3791
1	C	0.15	0/2813	0.46	0/3791
1	D	0.15	0/2802	0.47	0/3777
1	E	0.16	0/2813	0.45	0/3791
1	F	0.24	0/2813	0.53	0/3791
All	All	0.17	0/16867	0.47	0/22732

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2754	0	2722	82	0
1	B	2754	0	2722	85	0
1	C	2754	0	2719	85	1
1	D	2743	0	2709	70	2
1	E	2754	0	2722	83	1
1	F	2754	0	2722	123	0
2	A	43	0	30	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	43	0	30	8	0
2	C	43	0	30	2	0
2	D	43	0	30	3	0
2	E	43	0	30	4	0
2	F	43	0	30	6	0
3	A	7	0	0	0	0
3	B	9	0	0	0	0
3	C	15	0	0	3	0
3	D	12	0	0	3	0
3	E	13	0	0	1	0
3	F	20	0	0	5	0
All	All	16847	0	16496	518	2

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 16.

All (518) 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:57:GLN:HE22	1:B:133:SER:HB3	1.13	1.04
1:F:61:PHE:HZ	1:F:409:ILE:HD11	1.26	0.98
1:F:244:LEU:HD21	1:F:339:ARG:H	1.30	0.95
1:F:244:LEU:HD21	1:F:339:ARG:N	1.81	0.94
1:E:375:MET:HE2	2:E:501:HEM:HAC	1.49	0.91
1:B:249:ASP:O	1:B:251:THR:N	2.09	0.85
1:F:181:GLN:OE1	1:F:277:LYS:NZ	2.08	0.84
1:D:333:THR:HG21	1:D:375:MET:HG2	1.59	0.84
1:F:233:ARG:NH1	1:F:237:GLY:O	2.13	0.82
1:E:373:ILE:HG13	1:E:374:PRO:HD3	1.61	0.81
1:D:70:THR:HG22	1:D:253:MET:HE3	1.62	0.80
1:A:74:GLN:OE1	1:A:340:ARG:NH2	2.14	0.80
1:C:335:LYS:HG2	1:C:371:GLN:HG2	1.61	0.80
1:B:158:LEU:HD22	1:B:412:ARG:HH12	1.46	0.80
1:C:278:ILE:HG12	1:C:391:THR:HG22	1.65	0.79
1:D:100:THR:HG21	1:D:409:ILE:H	1.49	0.78
1:F:296:THR:HG21	1:F:388:TYR:HE2	1.48	0.77
1:F:287:ARG:NH2	3:F:601:HOH:O	2.16	0.77
1:F:371:GLN:O	1:F:375:MET:HG3	1.84	0.77
1:E:352:THR:HG22	1:E:354:TYR:HD2	1.48	0.77
1:C:309:GLN:NE2	1:C:315:PRO:O	2.16	0.76
1:F:214:GLU:O	1:F:215:VAL:HG23	1.85	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:ARG:NH1	2:B:501:HEM:HAD2	2.00	0.76
1:B:57:GLN:NE2	1:B:133:SER:HB3	1.97	0.74
1:F:84:VAL:HG11	1:F:92:ILE:HD11	1.69	0.74
1:E:412:ARG:C	1:E:414:LEU:H	1.96	0.74
1:F:404:LYS:HG2	1:F:405:LYS:H	1.53	0.73
1:B:233:ARG:NH1	1:B:301:LYS:O	2.21	0.73
1:F:74:GLN:OE1	1:F:340:ARG:NH2	2.22	0.72
1:A:318:LEU:HD11	1:A:331:LYS:HD3	1.70	0.72
1:D:196:GLN:HA	1:D:199:PHE:HB3	1.71	0.72
1:C:74:GLN:OE1	1:C:340:ARG:NH2	2.23	0.72
1:A:278:ILE:HG12	1:A:391:THR:HG22	1.71	0.71
1:A:322:PRO:HG2	1:A:325:SER:HB2	1.73	0.71
1:B:244:LEU:HD13	1:B:337:ILE:O	1.91	0.70
1:A:249:ASP:O	1:A:251:THR:N	2.24	0.70
1:F:316:VAL:HG11	1:F:327:VAL:HG11	1.72	0.69
1:E:404:LYS:HE2	1:E:406:GLY:H	1.56	0.69
1:D:74:GLN:OE1	1:D:340:ARG:NH2	2.26	0.69
1:A:195:GLU:N	1:F:76:TYR:OH	2.18	0.68
1:A:119:GLN:HB3	1:F:291:LYS:HB2	1.74	0.68
1:F:207:ASN:C	1:F:209:ALA:H	2.01	0.68
1:E:139:VAL:HG22	1:E:190:VAL:HG12	1.76	0.68
1:F:61:PHE:CZ	1:F:409:ILE:HD11	2.18	0.68
1:E:126:THR:OG1	1:E:204:ASN:OD1	2.11	0.68
1:C:233:ARG:NH1	1:C:301:LYS:O	2.22	0.67
1:F:146:GLY:O	1:F:155:ARG:NH1	2.28	0.67
1:B:242:THR:OG1	1:B:312:GLU:OE2	2.09	0.66
1:C:307:PHE:HB2	1:C:321:ILE:HG22	1.77	0.66
1:D:370:ASN:OD1	1:E:367:ASN:ND2	2.28	0.66
1:E:78:TYR:HB3	1:E:202:LEU:HD22	1.77	0.66
1:A:280:MET:HB2	1:A:358:GLY:HA2	1.78	0.66
1:A:78:TYR:HE1	1:F:345:THR:HG21	1.61	0.66
1:E:73:HIS:HE1	1:E:223:LEU:HB3	1.61	0.66
1:A:235:LEU:O	1:F:203:ARG:NH1	2.28	0.66
1:E:309:GLN:NE2	1:E:315:PRO:O	2.23	0.66
1:A:203:ARG:NH2	1:F:286:ASP:OD1	2.27	0.65
1:F:296:THR:HG22	1:F:384:ALA:HB1	1.78	0.65
1:F:307:PHE:HB2	1:F:321:ILE:HG22	1.79	0.65
1:B:245:GLN:HG3	1:B:252:LEU:HD13	1.78	0.64
1:E:412:ARG:O	1:E:414:LEU:N	2.30	0.64
1:A:103:THR:O	1:A:107:THR:OG1	2.15	0.64
1:A:373:ILE:HG22	1:A:377:LYS:HE3	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:GLU:HG2	1:A:57:GLN:H	1.61	0.64
1:F:78:TYR:HB3	1:F:202:LEU:HD22	1.80	0.64
1:D:259:ILE:HG12	1:D:366:LYS:HG3	1.80	0.64
1:F:215:VAL:O	1:F:217:PHE:N	2.29	0.64
1:A:289:SER:HA	1:F:122:PRO:HG3	1.80	0.63
1:C:254:ASN:HB3	1:C:260:GLN:HE21	1.63	0.63
1:D:277:LYS:HG3	1:D:392:ILE:HG13	1.80	0.63
1:D:206:LEU:HD13	1:D:215:VAL:HG21	1.81	0.63
1:F:276:ARG:HB2	1:F:361:PHE:HB3	1.81	0.63
1:F:412:ARG:HD3	1:F:413:LEU:H	1.62	0.63
1:B:102:LEU:HA	1:B:105:MET:HE3	1.81	0.62
1:B:235:LEU:O	1:C:203:ARG:NH2	2.28	0.62
1:C:254:ASN:HB3	1:C:260:GLN:NE2	2.13	0.62
1:C:78:TYR:HB3	1:C:202:LEU:HD22	1.82	0.62
1:C:89:LYS:NZ	1:C:413:LEU:O	2.29	0.62
1:E:330:ALA:O	1:E:333:THR:OG1	2.17	0.62
1:C:333:THR:HG21	1:C:375:MET:HG2	1.82	0.62
1:C:400:PRO:HG2	1:C:410:ALA:HB2	1.82	0.62
1:D:180:LYS:NZ	3:D:602:HOH:O	2.32	0.62
1:D:124:GLN:NE2	3:D:603:HOH:O	2.32	0.61
1:B:137:LEU:HD11	1:B:201:ALA:HB2	1.82	0.61
1:C:296:THR:HG21	1:C:388:TYR:HE2	1.65	0.61
1:E:409:ILE:HG13	1:E:410:ALA:H	1.65	0.61
1:F:244:LEU:HD12	1:F:244:LEU:N	2.14	0.61
1:A:139:VAL:HG22	1:A:190:VAL:HG12	1.83	0.61
2:E:501:HEM:HBC2	2:E:501:HEM:HMC2	1.81	0.61
1:A:76:TYR:OH	1:F:195:GLU:HB3	1.99	0.60
1:D:102:LEU:HD23	1:D:205:LEU:HD23	1.83	0.60
2:F:501:HEM:HMC2	2:F:501:HEM:HBC2	1.82	0.60
1:A:119:GLN:HA	1:F:290:LEU:HG	1.82	0.60
1:F:233:ARG:NH2	3:F:605:HOH:O	2.34	0.60
1:A:246:SER:C	1:A:248:LYS:H	2.09	0.60
1:C:352:THR:OG1	1:C:353:GLY:N	2.24	0.60
1:E:296:THR:HG22	1:E:384:ALA:HB1	1.83	0.60
1:C:154:ASP:OD2	1:C:157:GLY:N	2.31	0.60
1:B:78:TYR:HB3	1:B:202:LEU:HD22	1.82	0.60
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.83	0.60
1:D:108:SER:O	1:D:134:PRO:HG3	2.02	0.60
1:D:132:LEU:HD21	1:D:196:GLN:HE21	1.67	0.59
1:A:247:THR:HG22	1:A:253:MET:HE2	1.83	0.59
1:F:81:ALA:HA	1:F:187:CYS:HA	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:GLN:NE2	1:C:317:LYS:HE3	2.17	0.59
1:F:375:MET:HE2	2:F:501:HEM:HAC	1.84	0.59
1:F:375:MET:CE	2:F:501:HEM:HAC	2.33	0.59
1:B:412:ARG:HD3	1:B:413:LEU:N	2.17	0.59
1:C:259:ILE:HG21	1:C:263:GLU:CD	2.27	0.59
1:A:283:GLU:O	1:A:287:ARG:NE	2.35	0.59
1:F:100:THR:HB	1:F:409:ILE:HG12	1.85	0.59
1:F:266:TRP:HB3	1:F:412:ARG:HB3	1.84	0.59
1:C:299:ARG:NH1	1:C:304:GLY:O	2.36	0.58
1:D:278:ILE:HD11	1:D:361:PHE:HB2	1.83	0.58
1:F:259:ILE:HG12	1:F:366:LYS:HG3	1.85	0.58
1:D:56:GLU:O	1:D:57:GLN:HG2	2.04	0.58
1:E:309:GLN:CD	1:E:317:LYS:HE2	2.29	0.58
1:D:311:LYS:HG2	1:D:312:GLU:H	1.68	0.58
1:E:349:ASP:HB2	1:E:356:ASP:HB2	1.85	0.58
1:A:137:LEU:HD21	1:A:201:ALA:HB2	1.85	0.57
1:E:223:LEU:HG	1:E:232:PRO:HB2	1.86	0.57
1:E:296:THR:HG21	1:E:388:TYR:HE2	1.69	0.57
1:E:352:THR:HG22	1:E:354:TYR:CD2	2.34	0.57
1:E:56:GLU:N	1:E:56:GLU:OE1	2.37	0.57
1:F:207:ASN:O	1:F:209:ALA:N	2.37	0.57
1:D:125:ASP:OD1	1:D:200:HIS:NE2	2.30	0.57
1:F:82:LEU:N	1:F:186:ILE:O	2.28	0.57
1:B:294:GLU:OE1	1:B:300:ARG:NH1	2.37	0.57
1:A:246:SER:O	1:A:248:LYS:N	2.36	0.57
1:E:70:THR:HG22	1:E:253:MET:HE2	1.86	0.57
1:E:318:LEU:HD23	1:E:321:ILE:HD11	1.86	0.57
1:F:190:VAL:HG21	1:F:202:LEU:HB2	1.86	0.57
1:F:330:ALA:O	1:F:333:THR:OG1	2.22	0.56
1:E:283:GLU:OE1	1:E:283:GLU:N	2.31	0.56
1:F:192:ALA:C	1:F:194:ASP:H	2.13	0.56
1:F:194:ASP:OD1	1:F:196:GLN:NE2	2.37	0.56
1:F:293:GLN:O	1:F:296:THR:OG1	2.23	0.56
1:A:330:ALA:O	1:A:333:THR:OG1	2.23	0.56
1:D:102:LEU:HA	1:D:105:MET:HE2	1.87	0.56
1:E:308:GLY:O	1:E:317:LYS:NZ	2.29	0.56
1:A:99:TRP:NE1	1:A:205:LEU:O	2.36	0.56
1:A:412:ARG:HD2	1:A:412:ARG:N	2.20	0.56
1:F:144:GLY:N	1:F:185:ASP:O	2.29	0.56
1:E:61:PHE:CB	1:E:107:THR:HG21	2.36	0.56
1:F:296:THR:HG22	1:F:384:ALA:CB	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:TYR:HE2	1:A:195:GLU:HG3	1.70	0.56
1:D:270:GLY:N	1:D:401:GLY:HA2	2.21	0.56
1:C:118:ASN:HB3	1:C:121:LEU:HB2	1.88	0.55
1:F:139:VAL:HG22	1:F:190:VAL:HG12	1.87	0.55
1:E:412:ARG:C	1:E:414:LEU:N	2.65	0.55
1:E:100:THR:HG21	1:E:408:TYR:HA	1.88	0.55
1:F:360:LEU:HD23	1:F:360:LEU:H	1.71	0.55
1:C:56:GLU:O	1:C:56:GLU:HG2	2.06	0.55
1:A:100:THR:HG21	1:A:408:TYR:HA	1.88	0.55
1:C:233:ARG:NH1	1:C:237:GLY:O	2.32	0.55
1:E:266:TRP:HB3	1:E:412:ARG:CD	2.37	0.55
1:F:326:HIS:HA	1:F:379:LEU:HD21	1.88	0.55
1:A:78:TYR:HB3	1:A:202:LEU:HD22	1.89	0.54
1:D:342:PHE:O	1:D:360:LEU:N	2.29	0.54
1:C:84:VAL:O	1:C:85:THR:OG1	2.23	0.54
1:F:379:LEU:O	1:F:383:ASP:HB2	2.07	0.54
1:A:342:PHE:O	1:A:360:LEU:N	2.32	0.54
1:F:289:SER:O	1:F:293:GLN:HG3	2.07	0.54
1:B:296:THR:HG21	1:B:388:TYR:HE1	1.72	0.54
1:C:256:ILE:O	1:C:366:LYS:N	2.40	0.54
1:D:371:GLN:O	1:D:375:MET:HG3	2.08	0.54
1:A:253:MET:HE1	1:A:338:LEU:HD13	1.88	0.54
1:C:139:VAL:O	3:C:601:HOH:O	2.18	0.54
2:D:501:HEM:HMC1	2:D:501:HEM:HBC2	1.90	0.54
1:F:244:LEU:N	1:F:244:LEU:CD1	2.70	0.54
1:D:192:ALA:HB3	1:D:198:ALA:HB2	1.89	0.54
1:E:350:PRO:C	1:E:352:THR:H	2.16	0.54
1:F:413:LEU:HB3	3:F:608:HOH:O	2.07	0.54
1:A:233:ARG:NH1	1:A:237:GLY:O	2.40	0.53
1:A:70:THR:HG22	1:A:253:MET:HE3	1.90	0.53
2:A:501:HEM:HBC2	2:A:501:HEM:HMC1	1.90	0.53
1:F:58:ILE:HG21	1:F:108:SER:HA	1.88	0.53
1:F:361:PHE:HE1	1:F:372:PHE:HE2	1.57	0.53
1:A:311:LYS:HG2	1:A:312:GLU:H	1.73	0.53
1:B:103:THR:O	1:B:107:THR:OG1	2.23	0.53
1:D:187:CYS:HB3	1:D:397:TYR:CD1	2.44	0.53
1:B:339:ARG:HH12	2:B:501:HEM:HAD2	1.74	0.53
2:B:501:HEM:HMC1	2:B:501:HEM:HBC2	1.90	0.53
2:C:501:HEM:HBB2	2:C:501:HEM:HMB2	1.91	0.53
1:A:244:LEU:HG	1:A:338:LEU:HD12	1.91	0.53
1:C:56:GLU:OE1	1:C:56:GLU:N	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:PHE:N	1:D:343:SER:O	2.40	0.53
1:F:296:THR:HG21	1:F:388:TYR:CE2	2.37	0.53
1:D:99:TRP:NE1	1:D:205:LEU:O	2.41	0.52
1:A:156:PHE:HB2	1:A:158:LEU:HD12	1.90	0.52
1:B:254:ASN:HB3	1:B:260:GLN:HE22	1.74	0.52
1:A:408:TYR:CE1	1:A:411:GLN:HA	2.43	0.52
2:E:501:HEM:HBB2	2:E:501:HEM:HMB2	1.91	0.52
1:C:241:GLY:HA2	1:C:339:ARG:HH11	1.74	0.52
1:D:226:GLY:HA3	1:D:230:GLU:HG2	1.92	0.52
1:F:412:ARG:HD3	1:F:413:LEU:N	2.25	0.52
1:B:56:GLU:N	1:B:56:GLU:OE1	2.43	0.52
1:D:100:THR:HG21	1:D:408:TYR:HB2	1.92	0.52
1:F:278:ILE:HG12	1:F:391:THR:HG22	1.90	0.52
1:F:329:LEU:HD13	1:F:379:LEU:HA	1.92	0.52
1:E:85:THR:HG23	1:E:214:GLU:HB2	1.92	0.52
1:C:59:VAL:HG11	1:C:71:THR:HG21	1.91	0.52
1:D:264:PRO:HB2	1:D:266:TRP:CD1	2.45	0.52
1:A:102:LEU:HD23	1:A:205:LEU:HD23	1.92	0.51
1:C:254:ASN:O	1:C:260:GLN:NE2	2.32	0.51
1:C:89:LYS:HE3	1:C:158:LEU:HD21	1.91	0.51
1:C:158:LEU:HD22	1:C:161:LYS:HZ3	1.75	0.51
1:C:256:ILE:HG22	1:C:257:VAL:HG13	1.92	0.51
1:D:135:SER:HB3	1:D:193:ASP:HB2	1.92	0.51
1:A:120:TYR:C	1:F:289:SER:HB2	2.35	0.51
1:A:226:GLY:HA3	1:A:230:GLU:HB2	1.92	0.51
1:D:177:LEU:HD11	1:D:394:SER:HB3	1.92	0.51
2:F:501:HEM:HMB2	2:F:501:HEM:HBB2	1.92	0.51
1:F:183:GLY:H	1:F:395:ALA:HB2	1.76	0.51
1:A:267:MET:SD	1:A:398:ALA:HB1	2.50	0.51
1:C:310:LYS:HG3	1:C:311:LYS:HG3	1.92	0.51
1:D:246:SER:C	1:D:248:LYS:H	2.18	0.51
1:D:278:ILE:HD12	2:D:501:HEM:CAB	2.40	0.51
1:F:361:PHE:CE1	1:F:372:PHE:HE2	2.28	0.51
1:A:267:MET:HE1	1:A:272:TYR:CZ	2.46	0.51
1:B:126:THR:HG21	1:B:203:ARG:CZ	2.40	0.51
1:F:78:TYR:HE2	1:F:195:GLU:HG3	1.74	0.51
1:F:299:ARG:HD2	2:F:501:HEM:HBA1	1.93	0.51
1:B:179:GLU:HG2	1:B:216:ARG:HH21	1.75	0.51
1:E:150:LYS:HE3	1:E:155:ARG:HD3	1.93	0.51
1:A:224:SER:C	1:A:232:PRO:HB3	2.36	0.50
2:A:501:HEM:HBB2	2:A:501:HEM:HMB2	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:TYR:CD2	1:B:405:LYS:HD2	2.46	0.50
1:B:128:GLU:CD	1:B:203:ARG:HH21	2.20	0.50
1:E:61:PHE:HB3	1:E:107:THR:HG21	1.92	0.50
1:E:226:GLY:HA3	1:E:230:GLU:HB2	1.92	0.50
1:E:280:MET:HB2	1:E:358:GLY:HA2	1.94	0.50
1:A:132:LEU:HD23	1:A:197:VAL:HG23	1.94	0.50
1:B:412:ARG:HD3	1:B:413:LEU:H	1.76	0.50
1:D:132:LEU:HD23	1:D:197:VAL:HG23	1.94	0.50
2:D:501:HEM:HBB2	2:D:501:HEM:HMB2	1.94	0.50
1:B:62:TYR:HB3	1:B:404:LYS:O	2.12	0.50
1:D:333:THR:HG22	1:D:335:LYS:HG2	1.93	0.50
1:F:207:ASN:C	1:F:209:ALA:N	2.68	0.50
1:D:106:LEU:HD13	1:D:201:ALA:HA	1.94	0.50
2:B:501:HEM:HBB2	2:B:501:HEM:HMB2	1.93	0.50
1:F:149:GLU:OE2	1:F:159:LYS:NZ	2.28	0.50
1:E:99:TRP:HZ2	1:E:209:ALA:HB2	1.77	0.50
1:F:61:PHE:HB2	1:F:107:THR:HG21	1.94	0.50
1:E:289:SER:OG	1:E:290:LEU:N	2.45	0.49
1:A:131:ASP:O	1:F:227:LYS:N	2.45	0.49
1:A:173:PRO:O	1:A:380:SER:OG	2.30	0.49
1:C:280:MET:HB2	1:C:358:GLY:HA2	1.94	0.49
1:C:318:LEU:HD23	1:C:321:ILE:HD11	1.94	0.49
1:B:250:ASP:O	1:B:254:ASN:ND2	2.33	0.49
1:E:259:ILE:HD12	1:E:263:GLU:HG3	1.93	0.49
1:B:326:HIS:HD2	2:B:501:HEM:C1A	2.30	0.49
1:C:264:PRO:HB2	1:C:266:TRP:CD1	2.47	0.49
1:D:264:PRO:HB2	1:D:266:TRP:NE1	2.27	0.49
1:E:190:VAL:HG21	1:E:202:LEU:HB2	1.95	0.49
1:F:84:VAL:HG12	1:F:86:ALA:H	1.77	0.49
1:C:173:PRO:HB2	1:C:380:SER:O	2.13	0.49
1:D:266:TRP:HB3	1:D:412:ARG:CG	2.42	0.49
1:B:94:THR:O	1:B:98:ASN:ND2	2.37	0.49
1:B:190:VAL:HG11	1:B:201:ALA:HB3	1.95	0.49
1:B:412:ARG:HD3	1:B:413:LEU:HD12	1.94	0.49
1:A:284:VAL:HG22	1:A:287:ARG:HH11	1.78	0.49
1:D:256:ILE:HG13	1:D:257:VAL:HG23	1.94	0.49
1:E:92:ILE:HA	1:E:95:LEU:HD23	1.94	0.49
1:C:283:GLU:HG2	1:C:284:VAL:HG23	1.95	0.48
1:F:223:LEU:HG	1:F:232:PRO:HB2	1.95	0.48
1:F:237:GLY:HA3	1:F:301:LYS:HE2	1.96	0.48
1:D:195:GLU:O	1:D:199:PHE:N	2.40	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:GLU:HG2	1:D:284:VAL:HG23	1.94	0.48
1:F:207:ASN:C	1:F:208:GLN:HG3	2.38	0.48
1:B:375:MET:HE2	1:B:375:MET:HB3	1.70	0.48
1:C:100:THR:HG21	1:C:408:TYR:HA	1.95	0.48
1:E:234:ASN:ND2	1:E:240:ASP:OD1	2.44	0.48
1:F:99:TRP:CD1	1:F:205:LEU:HD22	2.48	0.48
1:F:65:HIS:ND1	1:F:269:GLY:O	2.38	0.48
1:B:118:ASN:HB3	1:B:121:LEU:HB2	1.95	0.48
1:D:314:ASP:OD2	3:D:601:HOH:O	2.20	0.48
1:F:284:VAL:HG12	1:F:287:ARG:HH11	1.78	0.48
1:B:100:THR:HG21	1:B:408:TYR:HA	1.95	0.48
1:F:267:MET:SD	1:F:398:ALA:HB1	2.53	0.48
1:B:283:GLU:HG2	1:B:284:VAL:HG13	1.95	0.48
1:E:94:THR:O	1:E:98:ASN:ND2	2.47	0.48
1:B:73:HIS:HE1	1:B:223:LEU:HB3	1.79	0.48
1:C:204:ASN:OD1	3:C:602:HOH:O	2.19	0.48
1:B:107:THR:HG23	1:B:137:LEU:O	2.14	0.48
1:A:165:HIS:HB2	1:A:272:TYR:CZ	2.49	0.47
1:C:89:LYS:HZ1	1:C:158:LEU:HD21	1.79	0.47
1:D:350:PRO:C	1:D:352:THR:H	2.22	0.47
1:F:73:HIS:HE1	1:F:223:LEU:HB3	1.79	0.47
1:D:143:PHE:O	1:D:398:ALA:N	2.36	0.47
1:A:224:SER:OG	1:F:196:GLN:NE2	2.46	0.47
1:E:172:MET:HE3	1:E:376:LEU:HD23	1.96	0.47
1:F:253:MET:HA	1:F:253:MET:HE2	1.95	0.47
1:D:242:THR:O	1:D:339:ARG:NH2	2.47	0.47
1:E:61:PHE:HB2	1:E:107:THR:HG21	1.96	0.47
1:A:246:SER:C	1:A:248:LYS:N	2.73	0.47
1:E:178:ASP:OD1	3:E:601:HOH:O	2.20	0.47
1:E:267:MET:HE1	1:E:398:ALA:HB1	1.96	0.47
1:A:73:HIS:ND1	1:A:74:GLN:O	2.47	0.47
1:B:158:LEU:HD22	1:B:412:ARG:NH1	2.24	0.47
1:B:349:ASP:HB3	1:B:352:THR:HB	1.96	0.47
1:C:296:THR:HG21	1:C:388:TYR:CE2	2.49	0.47
1:E:233:ARG:NH1	1:E:301:LYS:O	2.48	0.47
1:F:82:LEU:HG	1:F:215:VAL:HA	1.97	0.47
1:F:244:LEU:CD1	1:F:244:LEU:H	2.28	0.47
1:E:318:LEU:HA	1:E:321:ILE:HD11	1.96	0.47
1:F:280:MET:HE3	1:F:359:LEU:HB2	1.96	0.47
1:F:306:PRO:CB	1:F:316:VAL:HA	2.45	0.47
1:C:309:GLN:HE22	1:C:317:LYS:HE3	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:ASN:O	1:E:210:VAL:HG13	2.15	0.47
1:A:263:GLU:HG3	1:A:264:PRO:HD2	1.97	0.47
1:B:57:GLN:NE2	1:B:134:PRO:HD2	2.30	0.47
1:B:349:ASP:HB2	1:B:356:ASP:HB2	1.97	0.47
1:F:126:THR:OG1	1:F:128:GLU:OE1	2.33	0.47
1:F:194:ASP:OD1	1:F:196:GLN:CD	2.57	0.47
1:C:132:LEU:HD23	1:C:197:VAL:HG23	1.96	0.46
1:C:260:GLN:O	1:C:268:THR:HG23	2.16	0.46
1:E:276:ARG:HD2	1:E:372:PHE:HZ	1.81	0.46
1:A:56:GLU:HG2	1:A:57:GLN:N	2.28	0.46
1:A:254:ASN:HA	1:A:258:TRP:HB2	1.96	0.46
1:C:173:PRO:HG2	1:C:381:ALA:HB2	1.98	0.46
1:C:289:SER:O	1:C:293:GLN:HG3	2.15	0.46
1:E:246:SER:HB2	1:E:249:ASP:OD2	2.14	0.46
1:A:106:LEU:HD22	1:A:200:HIS:HE1	1.80	0.46
1:B:259:ILE:HG12	1:B:366:LYS:HG3	1.96	0.46
1:C:58:ILE:HG22	1:C:134:PRO:HG2	1.98	0.46
1:C:99:TRP:O	1:C:103:THR:HG22	2.16	0.46
1:E:242:THR:O	1:E:242:THR:HG23	2.15	0.46
1:D:71:THR:HG21	1:D:138:THR:HG21	1.98	0.46
1:D:118:ASN:HB3	1:D:121:LEU:HD13	1.97	0.46
1:D:252:LEU:O	1:D:256:ILE:HG12	2.14	0.46
1:A:290:LEU:HD13	1:F:123:PRO:HG3	1.96	0.46
1:B:207:ASN:O	1:B:210:VAL:HG13	2.16	0.46
1:B:89:LYS:HE2	1:B:89:LYS:HB3	1.79	0.46
1:A:225:GLY:O	1:F:132:LEU:HD21	2.16	0.46
1:E:138:THR:O	1:E:190:VAL:HA	2.16	0.46
1:F:192:ALA:C	1:F:194:ASP:N	2.74	0.46
1:F:323:SER:OG	1:F:382:LYS:NZ	2.47	0.46
1:C:315:PRO:HG2	1:C:317:LYS:HE2	1.98	0.46
1:E:249:ASP:OD2	1:E:252:LEU:HD12	2.15	0.46
1:F:324:ASN:ND2	1:F:384:ALA:HB2	2.31	0.46
1:B:218:VAL:HG22	1:C:348:LEU:HG	1.97	0.46
1:C:254:ASN:HA	1:C:258:TRP:HB2	1.98	0.46
1:B:252:LEU:O	1:B:256:ILE:HG13	2.15	0.45
1:B:372:PHE:O	1:B:375:MET:HG2	2.16	0.45
1:A:146:GLY:O	1:A:155:ARG:NH1	2.49	0.45
1:D:105:MET:HB3	1:D:110:LYS:HD2	1.99	0.45
1:E:410:ALA:C	1:E:412:ARG:H	2.24	0.45
1:D:279:LYS:NZ	1:D:349:ASP:OD2	2.49	0.45
1:C:327:VAL:O	1:C:331:LYS:HG2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:PHE:O	1:B:360:LEU:N	2.41	0.45
1:B:326:HIS:CE1	2:B:501:HEM:NC	2.78	0.45
1:C:158:LEU:HD22	1:C:161:LYS:NZ	2.31	0.45
1:D:367:ASN:C	1:D:367:ASN:HD22	2.25	0.45
1:E:73:HIS:CE1	1:E:223:LEU:HB3	2.47	0.45
1:E:289:SER:O	1:E:293:GLN:HG3	2.16	0.45
1:E:66:GLN:NE2	1:E:400:PRO:HG2	2.31	0.45
1:F:329:LEU:HD11	1:F:382:LYS:O	2.15	0.45
1:F:59:VAL:HG23	1:F:136:ASN:HA	1.97	0.45
1:F:96:PHE:HD2	1:F:413:LEU:HD11	1.81	0.45
1:A:291:LYS:HG3	1:A:295:ASP:OD2	2.17	0.45
1:C:162:LYS:NZ	1:C:166:LEU:O	2.49	0.45
1:A:78:TYR:CE2	1:A:195:GLU:HG3	2.49	0.45
1:A:244:LEU:HD11	1:A:339:ARG:O	2.17	0.44
1:A:263:GLU:HG2	1:A:267:MET:HE2	1.98	0.44
1:B:210:VAL:HG21	1:C:287:ARG:NH1	2.33	0.44
1:B:280:MET:O	1:B:282:LEU:HD13	2.16	0.44
1:E:326:HIS:HD2	2:E:501:HEM:C1A	2.35	0.44
1:E:142:GLY:HA2	1:E:399:CYS:HA	1.99	0.44
1:E:246:SER:C	1:E:248:LYS:H	2.25	0.44
1:F:412:ARG:HD3	1:F:413:LEU:HG	1.99	0.44
1:A:89:LYS:HE2	1:A:156:PHE:O	2.17	0.44
1:A:128:GLU:HG2	1:A:200:HIS:HB2	2.00	0.44
1:B:102:LEU:HD23	1:B:205:LEU:HD23	1.98	0.44
1:D:196:GLN:O	1:D:200:HIS:N	2.23	0.44
1:F:326:HIS:HD2	2:F:501:HEM:C1A	2.36	0.44
1:B:326:HIS:HD2	2:B:501:HEM:NA	2.15	0.44
1:C:102:LEU:HD23	1:C:205:LEU:HD23	1.99	0.44
1:D:296:THR:HG22	1:D:384:ALA:HB1	2.00	0.44
1:E:177:LEU:HD11	1:E:394:SER:HB3	2.00	0.44
1:B:277:LYS:HD3	1:B:392:ILE:HD11	2.00	0.44
1:E:73:HIS:CE1	1:E:223:LEU:HD23	2.52	0.44
1:B:67:ALA:O	1:B:140:THR:OG1	2.32	0.44
1:D:379:LEU:O	1:D:383:ASP:HB2	2.17	0.44
1:E:99:TRP:CZ2	1:E:209:ALA:HB2	2.53	0.44
1:E:404:LYS:HE3	1:E:405:LYS:HB3	1.99	0.44
1:A:231:THR:HG22	1:A:232:PRO:HD2	2.00	0.43
1:B:75:THR:HG22	1:B:224:SER:HA	2.00	0.43
1:B:238:PHE:CZ	1:B:301:LYS:HB3	2.53	0.43
1:C:244:LEU:HD21	1:C:338:LEU:HG	1.98	0.43
1:F:276:ARG:O	1:F:361:PHE:N	2.41	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:LYS:HB2	1:C:119:GLN:HG2	1.99	0.43
1:A:78:TYR:HB2	1:A:190:VAL:HG23	1.99	0.43
1:A:183:GLY:H	1:A:395:ALA:HB2	1.82	0.43
1:B:264:PRO:HB2	1:B:266:TRP:CD1	2.53	0.43
1:E:56:GLU:O	1:E:56:GLU:HG2	2.18	0.43
1:A:190:VAL:HG21	1:A:202:LEU:HB2	2.00	0.43
1:B:296:THR:HG22	1:B:384:ALA:HB1	2.00	0.43
1:B:412:ARG:CD	1:B:413:LEU:HD12	2.48	0.43
1:C:294:GLU:HB3	1:C:307:PHE:HZ	1.84	0.43
1:E:62:TYR:CE2	1:E:405:LYS:HD2	2.52	0.43
1:F:67:ALA:HB3	3:F:620:HOH:O	2.17	0.43
1:C:242:THR:HG21	1:C:312:GLU:HB2	2.01	0.43
1:F:306:PRO:HB3	1:F:316:VAL:HA	2.01	0.43
1:C:58:ILE:HB	1:C:107:THR:O	2.18	0.43
1:D:70:THR:HG21	1:D:258:TRP:HE1	1.83	0.43
1:B:111:LYS:HE2	1:B:132:LEU:O	2.18	0.43
1:B:206:LEU:HD13	1:B:215:VAL:HG21	2.01	0.43
1:D:99:TRP:HZ2	1:D:209:ALA:HB2	1.81	0.43
1:D:111:LYS:HD3	1:D:130:ALA:HA	2.00	0.43
1:D:256:ILE:HG13	1:D:257:VAL:CG2	2.48	0.43
1:E:109:GLY:HA2	1:E:111:LYS:NZ	2.34	0.43
1:C:294:GLU:HB3	1:C:307:PHE:CZ	2.54	0.43
1:C:335:LYS:HD2	1:C:335:LYS:HA	1.71	0.43
1:E:150:LYS:HE3	1:E:150:LYS:HB3	1.72	0.43
1:F:132:LEU:HD13	1:F:196:GLN:HG3	2.00	0.43
1:A:61:PHE:HD2	1:A:104:GLN:HG2	1.84	0.43
1:A:307:PHE:HB2	1:A:321:ILE:HG22	2.01	0.43
1:B:74:GLN:OE1	1:B:340:ARG:NH2	2.51	0.43
1:B:243:GLY:HA3	2:B:501:HEM:O2D	2.19	0.43
1:D:146:GLY:O	1:D:155:ARG:NH2	2.52	0.43
1:D:164:LYS:HA	1:D:164:LYS:HD3	1.86	0.43
1:E:271:THR:OG1	1:E:365:GLN:O	2.35	0.43
1:B:350:PRO:C	1:B:352:THR:H	2.26	0.43
1:C:404:LYS:HG3	1:C:405:LYS:N	2.34	0.43
1:F:89:LYS:HB3	1:F:89:LYS:HE2	1.78	0.43
1:F:100:THR:HG21	1:F:408:TYR:HB2	2.01	0.43
1:F:128:GLU:HG2	1:F:200:HIS:HB2	2.01	0.43
1:B:355:MET:HE2	1:C:199:PHE:HE1	1.83	0.42
1:C:316:VAL:C	1:C:317:LYS:HD3	2.44	0.42
1:D:266:TRP:CD1	1:D:266:TRP:H	2.37	0.42
1:F:177:LEU:HD23	1:F:177:LEU:HA	1.79	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:ASN:HB3	1:B:260:GLN:NE2	2.33	0.42
1:B:412:ARG:HH11	1:B:413:LEU:N	2.17	0.42
1:C:274:ALA:O	1:C:362:ILE:HA	2.19	0.42
1:C:383:ASP:OD2	1:C:384:ALA:N	2.52	0.42
1:E:337:ILE:HD13	1:E:375:MET:SD	2.59	0.42
1:A:100:THR:OG1	1:A:409:ILE:HG12	2.19	0.42
1:B:132:LEU:HD11	1:B:196:GLN:HE21	1.83	0.42
1:E:158:LEU:HD21	1:E:413:LEU:HA	2.01	0.42
1:E:266:TRP:HB3	1:E:412:ARG:HD2	1.99	0.42
1:F:61:PHE:HD1	3:F:620:HOH:O	2.02	0.42
1:F:276:ARG:NH2	1:F:391:THR:HG21	2.34	0.42
1:F:341:ALA:HA	1:F:362:ILE:HG23	1.99	0.42
1:A:76:TYR:CE1	1:A:222:PHE:HB2	2.54	0.42
1:B:408:TYR:CZ	1:B:411:GLN:HG3	2.54	0.42
1:C:223:LEU:HG	1:C:232:PRO:HB2	2.02	0.42
1:E:96:PHE:CZ	1:E:186:ILE:HD13	2.55	0.42
1:F:316:VAL:HG23	1:F:331:LYS:NZ	2.35	0.42
1:B:408:TYR:CE2	1:B:411:GLN:HG3	2.55	0.42
1:C:257:VAL:HG12	1:C:364:PHE:O	2.20	0.42
1:F:66:GLN:NE2	1:F:400:PRO:HG2	2.35	0.42
1:B:279:LYS:NZ	1:B:349:ASP:OD1	2.43	0.42
1:B:312:GLU:HG2	1:B:313:THR:N	2.35	0.42
1:C:267:MET:SD	1:C:398:ALA:HB1	2.59	0.42
1:E:79:PHE:O	1:E:218:VAL:HA	2.20	0.42
1:F:172:MET:HB3	1:F:380:SER:OG	2.19	0.42
1:C:126:THR:N	3:C:602:HOH:O	2.53	0.41
1:C:256:ILE:HD13	1:C:336:GLN:HB2	2.01	0.41
1:D:99:TRP:CZ2	1:D:209:ALA:HB2	2.55	0.41
1:F:264:PRO:HB2	1:F:266:TRP:CD1	2.55	0.41
1:A:61:PHE:CD2	1:A:104:GLN:HG2	2.55	0.41
1:B:91:ASP:O	1:B:94:THR:OG1	2.32	0.41
1:B:266:TRP:CG	1:B:412:ARG:HG2	2.55	0.41
1:C:89:LYS:CE	1:C:158:LEU:HD21	2.49	0.41
1:C:89:LYS:HE2	1:C:413:LEU:HB3	2.03	0.41
1:F:404:LYS:HG2	1:F:405:LYS:N	2.28	0.41
1:B:122:PRO:HA	1:B:123:PRO:HD3	1.91	0.41
1:B:259:ILE:HA	1:B:366:LYS:HE3	2.02	0.41
1:C:78:TYR:HE2	1:C:195:GLU:HG3	1.85	0.41
1:E:336:GLN:O	1:E:337:ILE:HD12	2.21	0.41
1:E:410:ALA:O	1:E:412:ARG:N	2.51	0.41
1:F:81:ALA:HB3	1:F:217:PHE:CZ	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:259:ILE:HD13	1:F:263:GLU:OE2	2.20	0.41
1:C:89:LYS:NZ	1:C:158:LEU:HD21	2.35	0.41
1:D:246:SER:O	1:D:248:LYS:N	2.54	0.41
1:B:280:MET:HE2	1:B:358:GLY:HA2	2.02	0.41
1:C:126:THR:HG21	1:C:203:ARG:CZ	2.50	0.41
1:E:253:MET:HE3	1:E:253:MET:HB3	1.73	0.41
1:F:78:TYR:CE2	1:F:199:PHE:HB2	2.55	0.41
1:A:163:PRO:HG3	1:A:266:TRP:CZ2	2.56	0.41
1:B:93:ILE:HD13	1:B:414:LEU:HD23	2.02	0.41
1:B:142:GLY:HA2	1:B:399:CYS:HA	2.03	0.41
1:C:409:ILE:O	1:C:410:ALA:C	2.63	0.41
1:A:80:ALA:HB2	1:A:202:LEU:HD11	2.02	0.41
1:A:82:LEU:HD11	1:A:206:LEU:HD22	2.02	0.41
1:A:276:ARG:HH11	1:A:394:SER:HB2	1.86	0.41
1:B:247:THR:HA	1:B:253:MET:HE3	2.03	0.41
1:D:280:MET:HB2	1:D:358:GLY:HA2	2.02	0.41
1:E:373:ILE:CG1	1:E:374:PRO:HD3	2.43	0.41
1:F:206:LEU:HD22	1:F:215:VAL:HG22	2.03	0.41
1:A:74:GLN:NE2	1:A:138:THR:OG1	2.54	0.41
1:A:108:SER:O	1:A:134:PRO:HG3	2.20	0.41
1:B:218:VAL:HG21	1:C:355:MET:SD	2.61	0.41
1:B:348:LEU:HD11	1:C:215:VAL:HG12	2.03	0.41
1:C:379:LEU:O	1:C:383:ASP:HB2	2.21	0.41
1:D:178:ASP:HB3	1:D:181:GLN:HB2	2.03	0.41
1:F:266:TRP:HE3	1:F:400:PRO:HB3	1.84	0.41
1:F:267:MET:HE2	1:F:267:MET:HB3	1.97	0.41
1:F:318:LEU:HG	1:F:321:ILE:HD11	2.02	0.41
1:A:119:GLN:CB	1:F:291:LYS:HB2	2.46	0.41
1:C:149:GLU:OE2	1:C:152:GLY:HA2	2.21	0.41
1:E:365:GLN:OE1	1:E:372:PHE:HB2	2.21	0.41
1:F:133:SER:O	1:F:197:VAL:HG21	2.21	0.41
1:D:296:THR:HG21	1:D:388:TYR:HE2	1.86	0.40
1:D:412:ARG:HD3	1:D:412:ARG:HA	1.75	0.40
1:E:379:LEU:O	1:E:383:ASP:HB2	2.21	0.40
1:F:238:PHE:CE2	1:F:301:LYS:HE3	2.56	0.40
1:D:383:ASP:OD2	1:D:384:ALA:N	2.54	0.40
1:E:75:THR:O	1:E:222:PHE:HA	2.20	0.40
1:E:409:ILE:HG13	1:E:410:ALA:N	2.35	0.40
1:A:178:ASP:HB3	1:A:181:GLN:HB2	2.02	0.40
1:A:337:ILE:HG13	1:A:339:ARG:HG2	2.03	0.40
1:B:106:LEU:HD13	1:B:201:ALA:HA	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:HIS:HD2	1:C:340:ARG:HG3	1.85	0.40
1:F:285:TRP:HE3	1:F:388:TYR:CG	2.40	0.40
1:D:93:ILE:HG23	1:D:408:TYR:OH	2.22	0.40
1:D:248:LYS:H	1:D:248:LYS:HG2	1.78	0.40

All (2) 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)
1:D:194:ASP:O	1:E:76:TYR:OH[1_565]	2.09	0.11
1:C:324:ASN:ND2	1:D:120:TYR:O[4_547]	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	350/359 (98%)	321 (92%)	23 (7%)	6 (2%)	7	17
1	B	350/359 (98%)	326 (93%)	21 (6%)	3 (1%)	14	31
1	C	350/359 (98%)	330 (94%)	12 (3%)	8 (2%)	5	11
1	D	349/359 (97%)	322 (92%)	17 (5%)	10 (3%)	3	8
1	E	350/359 (98%)	321 (92%)	21 (6%)	8 (2%)	5	11
1	F	350/359 (98%)	316 (90%)	25 (7%)	9 (3%)	4	9
All	All	2099/2154 (97%)	1936 (92%)	119 (6%)	44 (2%)	5	13

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	247	THR
1	A	250	ASP
1	B	250	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	86	ALA
1	D	177	LEU
1	D	195	GLU
1	D	247	THR
1	F	208	GLN
1	F	215	VAL
1	F	216	ARG
1	A	245	GLN
1	A	251	THR
1	C	57	GLN
1	C	154	ASP
1	D	57	GLN
1	D	246	SER
1	D	410	ALA
1	D	413	LEU
1	E	86	ALA
1	E	246	SER
1	F	350	PRO
1	F	413	LEU
1	B	241	GLY
1	B	405	LYS
1	C	410	ALA
1	E	317	LYS
1	E	401	GLY
1	E	405	LYS
1	F	246	SER
1	A	241	GLY
1	C	241	GLY
1	C	245	GLN
1	E	247	THR
1	F	88	ASP
1	F	241	GLY
1	F	317	LYS
1	A	86	ALA
1	C	155	ARG
1	C	411	GLN
1	D	231	THR
1	D	401	GLY
1	E	57	GLN
1	E	243	GLY
1	C	84	VAL

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	296/300 (99%)	280 (95%)	16 (5%)	20	42
1	B	296/300 (99%)	285 (96%)	11 (4%)	30	56
1	C	296/300 (99%)	286 (97%)	10 (3%)	32	59
1	D	295/300 (98%)	277 (94%)	18 (6%)	17	37
1	E	296/300 (99%)	275 (93%)	21 (7%)	13	30
1	F	296/300 (99%)	275 (93%)	21 (7%)	13	30
All	All	1775/1800 (99%)	1678 (94%)	97 (6%)	19	41

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	VAL
1	A	107	THR
1	A	119	GLN
1	A	120	TYR
1	A	210	VAL
1	A	215	VAL
1	A	231	THR
1	A	244	LEU
1	A	251	THR
1	A	257	VAL
1	A	260	GLN
1	A	284	VAL
1	A	327	VAL
1	A	333	THR
1	A	365	GLN
1	A	392	ILE
1	B	71	THR
1	B	92	ILE
1	B	107	THR
1	B	210	VAL
1	B	247	THR
1	B	257	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	267	MET
1	B	282	LEU
1	B	313	THR
1	B	316	VAL
1	B	412	ARG
1	C	59	VAL
1	C	92	ILE
1	C	203	ARG
1	C	245	GLN
1	C	290	LEU
1	C	312	GLU
1	C	337	ILE
1	C	338	LEU
1	C	352	THR
1	C	392	ILE
1	D	84	VAL
1	D	88	ASP
1	D	92	ILE
1	D	104	GLN
1	D	118	ASN
1	D	124	GLN
1	D	230	GLU
1	D	248	LYS
1	D	257	VAL
1	D	260	GLN
1	D	273	MET
1	D	278	ILE
1	D	290	LEU
1	D	316	VAL
1	D	318	LEU
1	D	362	ILE
1	D	367	ASN
1	D	392	ILE
1	E	59	VAL
1	E	94	THR
1	E	95	LEU
1	E	126	THR
1	E	206	LEU
1	E	210	VAL
1	E	220	LYS
1	E	242	THR
1	E	247	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	248	LYS
1	E	259	ILE
1	E	267	MET
1	E	289	SER
1	E	316	VAL
1	E	321	ILE
1	E	327	VAL
1	E	333	THR
1	E	337	ILE
1	E	365	GLN
1	E	373	ILE
1	E	412	ARG
1	F	58	ILE
1	F	150	LYS
1	F	179	GLU
1	F	180	LYS
1	F	208	GLN
1	F	245	GLN
1	F	289	SER
1	F	290	LEU
1	F	311	LYS
1	F	316	VAL
1	F	317	LYS
1	F	318	LEU
1	F	327	VAL
1	F	333	THR
1	F	345	THR
1	F	360	LEU
1	F	362	ILE
1	F	365	GLN
1	F	375	MET
1	F	377	LYS
1	F	412	ARG

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	165	HIS
1	A	324	ASN
1	B	57	GLN
1	B	66	GLN
1	C	98	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	119	GLN
1	C	189	GLN
1	C	196	GLN
1	C	219	ASN
1	C	367	ASN
1	D	219	ASN
1	D	260	GLN
1	D	370	ASN
1	E	73	HIS
1	E	189	GLN
1	E	367	ASN
1	F	57	GLN
1	F	136	ASN
1	F	200	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	B	501	1	50,50,50	1.52	8 (16%)	66,82,82	1.43	6 (9%)
2	HEM	A	501	1	50,50,50	1.38	8 (16%)	66,82,82	1.18	4 (6%)
2	HEM	F	501	1	50,50,50	1.59	10 (20%)	66,82,82	1.36	9 (13%)
2	HEM	C	501	1	50,50,50	1.44	8 (16%)	66,82,82	1.16	6 (9%)
2	HEM	E	501	1	50,50,50	1.41	8 (16%)	66,82,82	1.20	7 (10%)
2	HEM	D	501	1	50,50,50	1.38	7 (14%)	66,82,82	1.23	7 (10%)

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	B	501	1	-	4/14/54/54	-
2	HEM	A	501	1	-	4/14/54/54	-
2	HEM	F	501	1	-	4/14/54/54	-
2	HEM	C	501	1	-	4/14/54/54	-
2	HEM	E	501	1	-	4/14/54/54	-
2	HEM	D	501	1	-	4/14/54/54	-

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	HEM	FE-ND	5.16	2.10	1.94
2	F	501	HEM	FE-NB	4.59	2.09	1.94
2	B	501	HEM	FE-NB	4.24	2.08	1.94
2	B	501	HEM	FE-ND	3.77	2.06	1.94
2	C	501	HEM	FE-NB	3.70	2.06	1.94
2	C	501	HEM	FE-ND	3.59	2.06	1.94
2	E	501	HEM	FE-NB	3.57	2.05	1.94
2	B	501	HEM	FE-NC	3.44	2.06	1.95
2	A	501	HEM	FE-ND	3.39	2.05	1.94
2	A	501	HEM	FE-NB	3.39	2.05	1.94
2	E	501	HEM	FE-ND	3.33	2.05	1.94
2	D	501	HEM	FE-NB	3.28	2.05	1.94
2	D	501	HEM	FE-NA	3.18	2.05	1.95
2	B	501	HEM	FE-NA	3.14	2.05	1.95
2	E	501	HEM	FE-NA	3.12	2.05	1.95
2	C	501	HEM	FE-NA	3.09	2.05	1.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	CAC-C3C	3.06	1.55	1.47
2	D	501	HEM	CAC-C3C	3.06	1.55	1.47
2	E	501	HEM	CAB-C3B	3.05	1.55	1.47
2	A	501	HEM	CAB-C3B	3.04	1.55	1.47
2	A	501	HEM	CAC-C3C	3.03	1.55	1.47
2	F	501	HEM	CAB-C3B	3.02	1.55	1.47
2	B	501	HEM	CAB-C3B	3.00	1.55	1.47
2	D	501	HEM	FE-ND	2.99	2.04	1.94
2	C	501	HEM	CAB-C3B	2.98	1.55	1.47
2	E	501	HEM	CAC-C3C	2.98	1.55	1.47
2	F	501	HEM	CAC-C3C	2.97	1.55	1.47
2	B	501	HEM	CAC-C3C	2.93	1.55	1.47
2	C	501	HEM	FE-NC	2.92	2.05	1.95
2	D	501	HEM	CAB-C3B	2.87	1.55	1.47
2	F	501	HEM	FE-NA	2.84	2.04	1.95
2	A	501	HEM	FE-NC	2.70	2.04	1.95
2	E	501	HEM	FE-NC	2.66	2.04	1.95
2	A	501	HEM	FE-NA	2.59	2.03	1.95
2	D	501	HEM	FE-NC	2.52	2.03	1.95
2	F	501	HEM	FE-NC	2.47	2.03	1.95
2	F	501	HEM	CMD-C2D	2.20	1.55	1.50
2	F	501	HEM	C2A-C3A	-2.18	1.33	1.38
2	F	501	HEM	CMC-C2C	2.17	1.55	1.50
2	A	501	HEM	CMB-C2B	2.09	1.55	1.50
2	A	501	HEM	CMC-C2C	2.08	1.55	1.50
2	B	501	HEM	CMD-C2D	2.07	1.55	1.50
2	B	501	HEM	CMB-C2B	2.06	1.55	1.50
2	F	501	HEM	CMB-C2B	2.06	1.55	1.50
2	E	501	HEM	CMB-C2B	2.06	1.55	1.50
2	C	501	HEM	CMB-C2B	2.04	1.55	1.50
2	C	501	HEM	CMC-C2C	2.04	1.55	1.50
2	E	501	HEM	CMC-C2C	2.03	1.55	1.50
2	D	501	HEM	CMB-C2B	2.00	1.55	1.50

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	CAD-CBD-CGD	-7.48	97.50	113.60
2	F	501	HEM	C4C-NC-C1C	4.24	109.50	105.35
2	F	501	HEM	CHD-C1D-C2D	3.32	130.16	124.98
2	D	501	HEM	C4D-ND-C1D	3.13	108.30	105.07
2	D	501	HEM	C4C-NC-C1C	3.10	108.38	105.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	HEM	C4C-NC-C1C	3.07	108.36	105.35
2	E	501	HEM	C4D-ND-C1D	3.05	108.22	105.07
2	A	501	HEM	C4D-ND-C1D	2.93	108.10	105.07
2	F	501	HEM	C4D-ND-C1D	2.93	108.10	105.07
2	A	501	HEM	C4A-NA-C1A	2.93	108.21	105.35
2	C	501	HEM	C4D-ND-C1D	2.92	108.09	105.07
2	D	501	HEM	C4A-NA-C1A	2.91	108.20	105.35
2	D	501	HEM	C1B-NB-C4B	2.90	108.06	105.07
2	A	501	HEM	C4C-NC-C1C	2.88	108.17	105.35
2	E	501	HEM	C4A-NA-C1A	2.87	108.16	105.35
2	E	501	HEM	C1B-NB-C4B	2.86	108.03	105.07
2	C	501	HEM	C4C-NC-C1C	2.84	108.13	105.35
2	F	501	HEM	C4C-C3C-C2C	2.81	109.06	106.75
2	A	501	HEM	C1B-NB-C4B	2.78	107.94	105.07
2	C	501	HEM	C4A-NA-C1A	2.77	108.06	105.35
2	C	501	HEM	C1B-NB-C4B	2.69	107.85	105.07
2	B	501	HEM	CHA-C4D-ND	2.66	127.65	124.37
2	B	501	HEM	C1B-NB-C4B	2.50	107.65	105.07
2	D	501	HEM	CAA-CBA-CGA	-2.47	108.28	113.60
2	C	501	HEM	CAD-CBD-CGD	-2.47	108.28	113.60
2	F	501	HEM	CAD-CBD-CGD	-2.43	108.37	113.60
2	B	501	HEM	C4A-NA-C1A	2.43	107.73	105.35
2	B	501	HEM	C4C-NC-C1C	2.36	107.66	105.35
2	F	501	HEM	C4A-C3A-C2A	2.32	109.55	106.83
2	F	501	HEM	CMD-C2D-C1D	2.30	128.54	125.04
2	F	501	HEM	C1B-NB-C4B	2.26	107.41	105.07
2	F	501	HEM	C2D-C1D-ND	-2.18	107.27	109.88
2	D	501	HEM	C2A-C1A-NA	-2.15	107.75	110.15
2	D	501	HEM	C3D-C4D-ND	-2.08	107.85	110.17
2	C	501	HEM	C2A-C1A-NA	-2.04	107.87	110.15
2	E	501	HEM	C3B-C2B-C1B	2.03	108.00	106.49
2	E	501	HEM	C2D-C1D-ND	-2.03	107.45	109.88
2	E	501	HEM	CAD-CBD-CGD	-2.02	109.26	113.60
2	B	501	HEM	C3D-C4D-ND	-2.01	107.93	110.17

There are no chirality outliers.

All (24) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	501	HEM	CAA-CBA-CGA-O1A
2	F	501	HEM	CAD-CBD-CGD-O1D
2	B	501	HEM	CAD-CBD-CGD-O2D
2	F	501	HEM	CAD-CBD-CGD-O2D
2	A	501	HEM	CAD-CBD-CGD-O2D
2	B	501	HEM	CAA-CBA-CGA-O1A
2	F	501	HEM	CAA-CBA-CGA-O1A
2	C	501	HEM	CAA-CBA-CGA-O1A
2	E	501	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	CAA-CBA-CGA-O1A
2	C	501	HEM	CAD-CBD-CGD-O1D
2	C	501	HEM	CAD-CBD-CGD-O2D
2	D	501	HEM	CAD-CBD-CGD-O2D
2	E	501	HEM	CAD-CBD-CGD-O2D
2	D	501	HEM	CAA-CBA-CGA-O2A
2	B	501	HEM	CAA-CBA-CGA-O2A
2	B	501	HEM	CAD-CBD-CGD-O1D
2	C	501	HEM	CAA-CBA-CGA-O2A
2	F	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	CAA-CBA-CGA-O2A
2	E	501	HEM	CAA-CBA-CGA-O2A

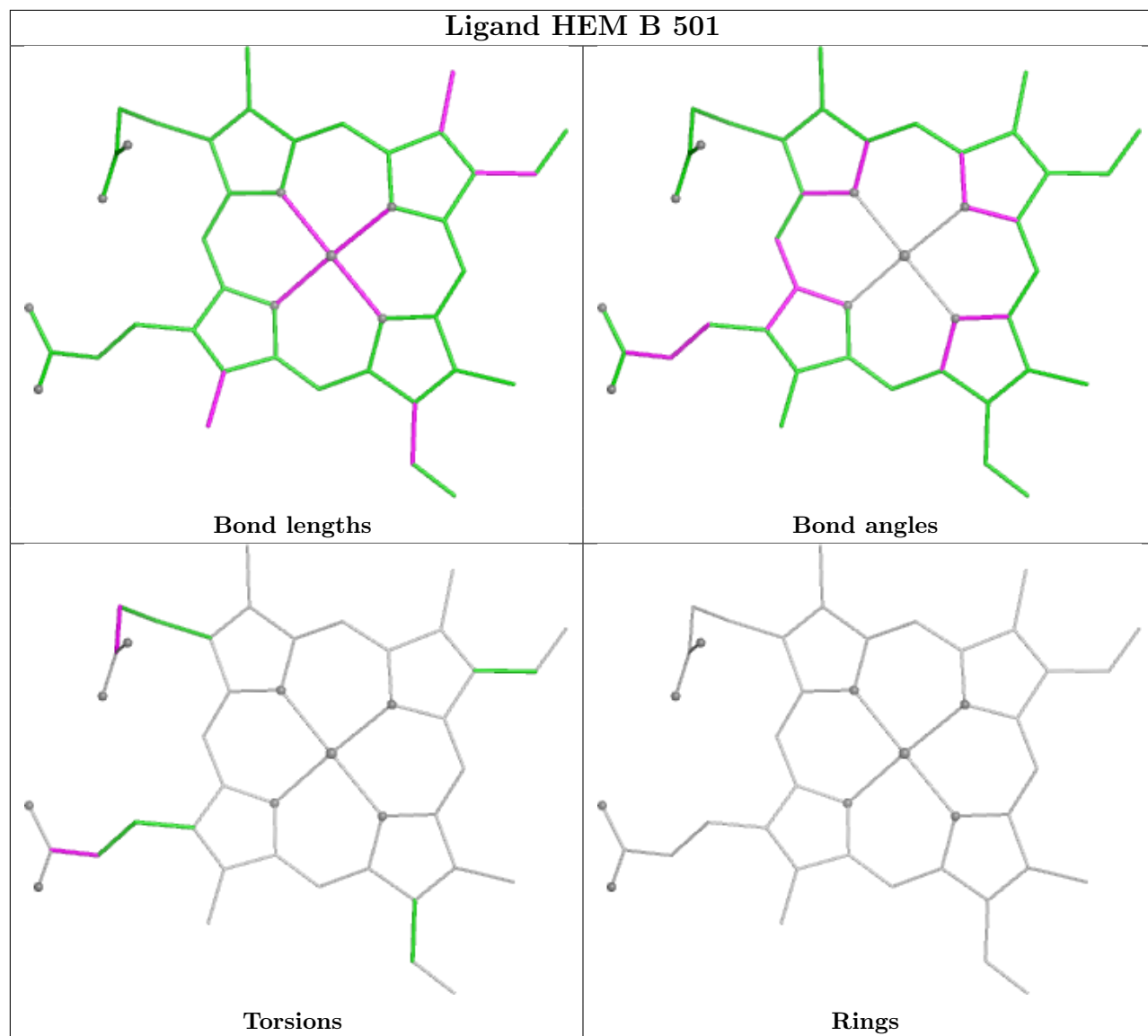
There are no ring outliers.

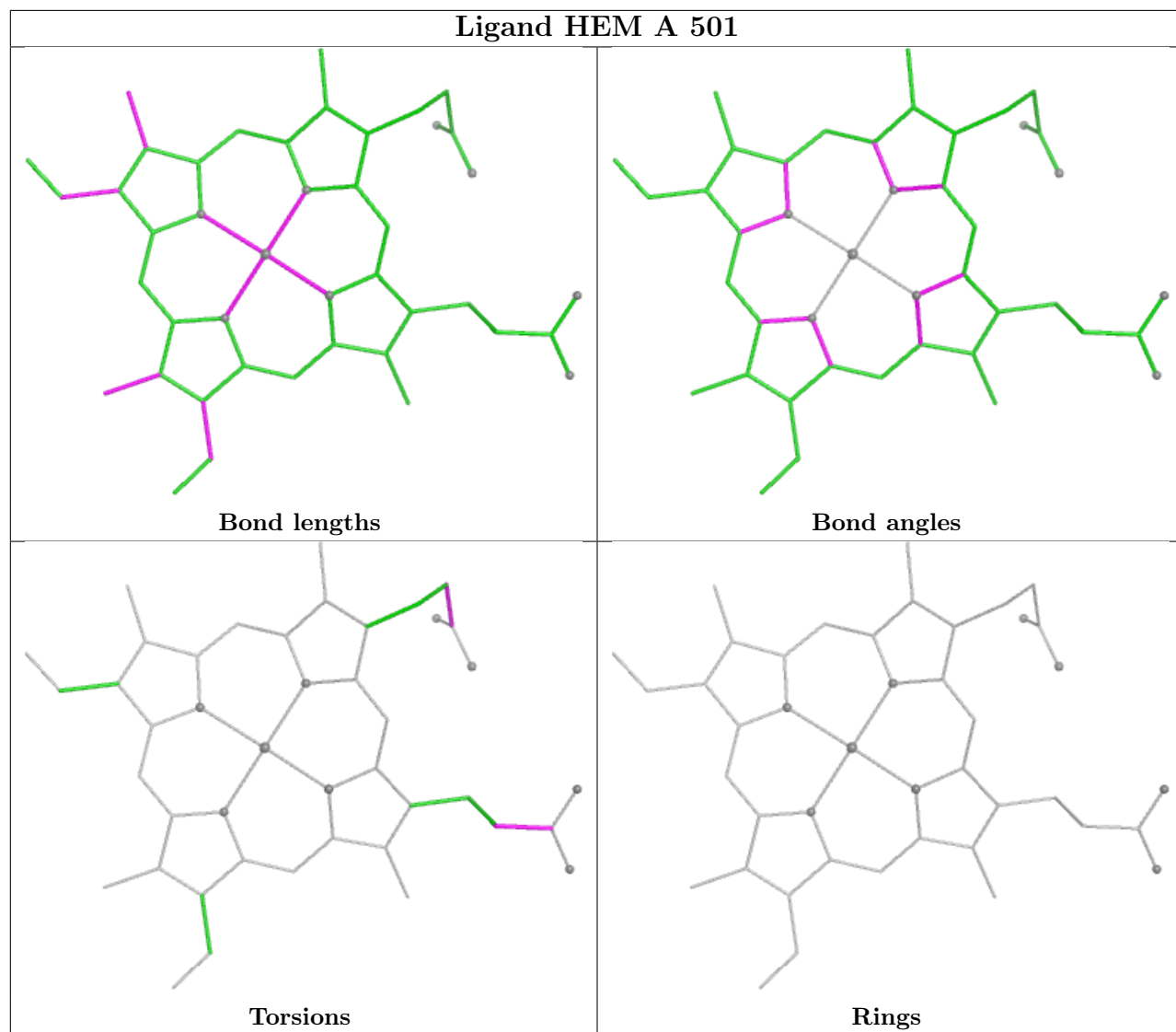
6 monomers are involved in 25 short contacts:

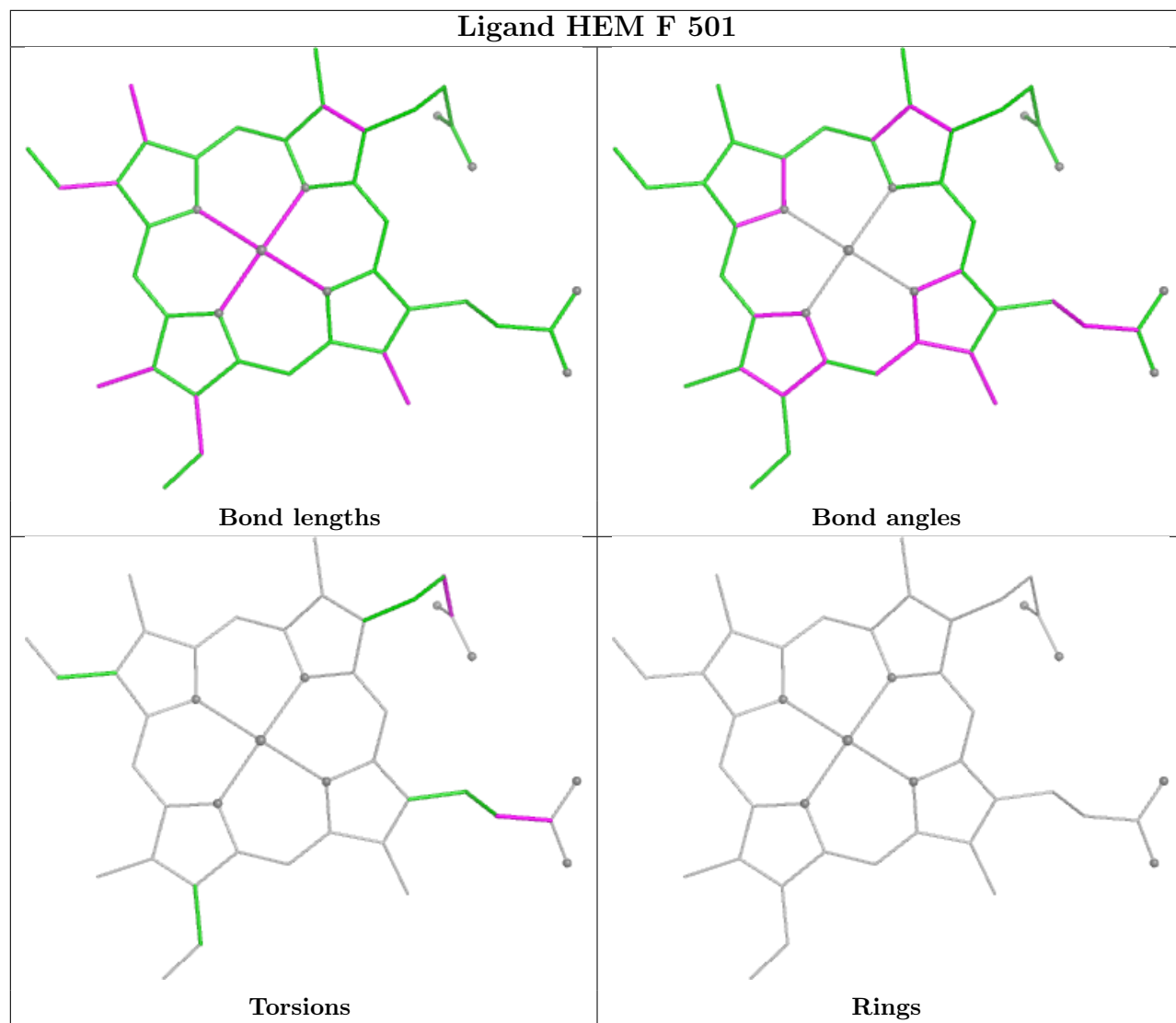
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	HEM	8	0
2	A	501	HEM	2	0
2	F	501	HEM	6	0
2	C	501	HEM	2	0
2	E	501	HEM	4	0
2	D	501	HEM	3	0

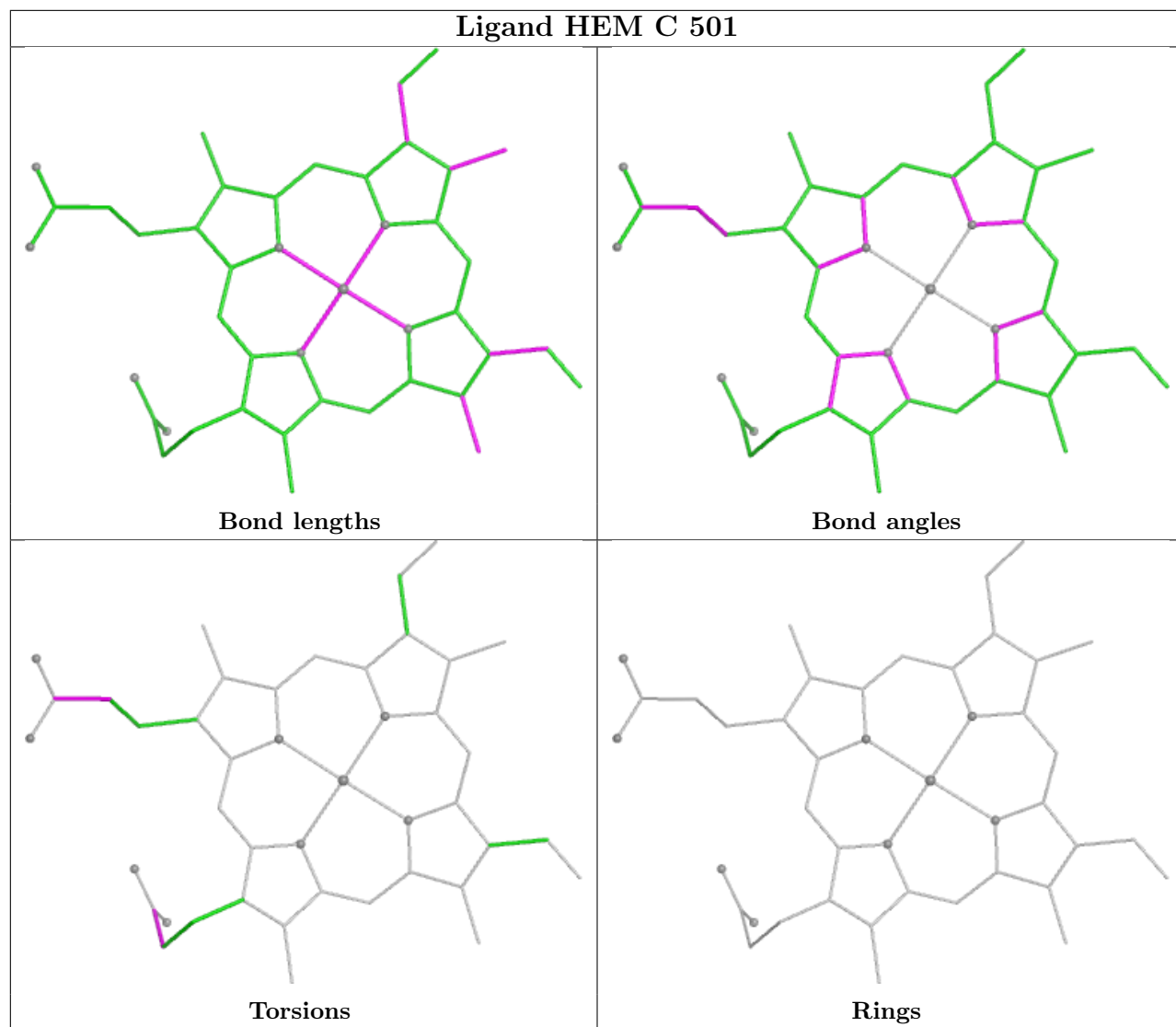
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

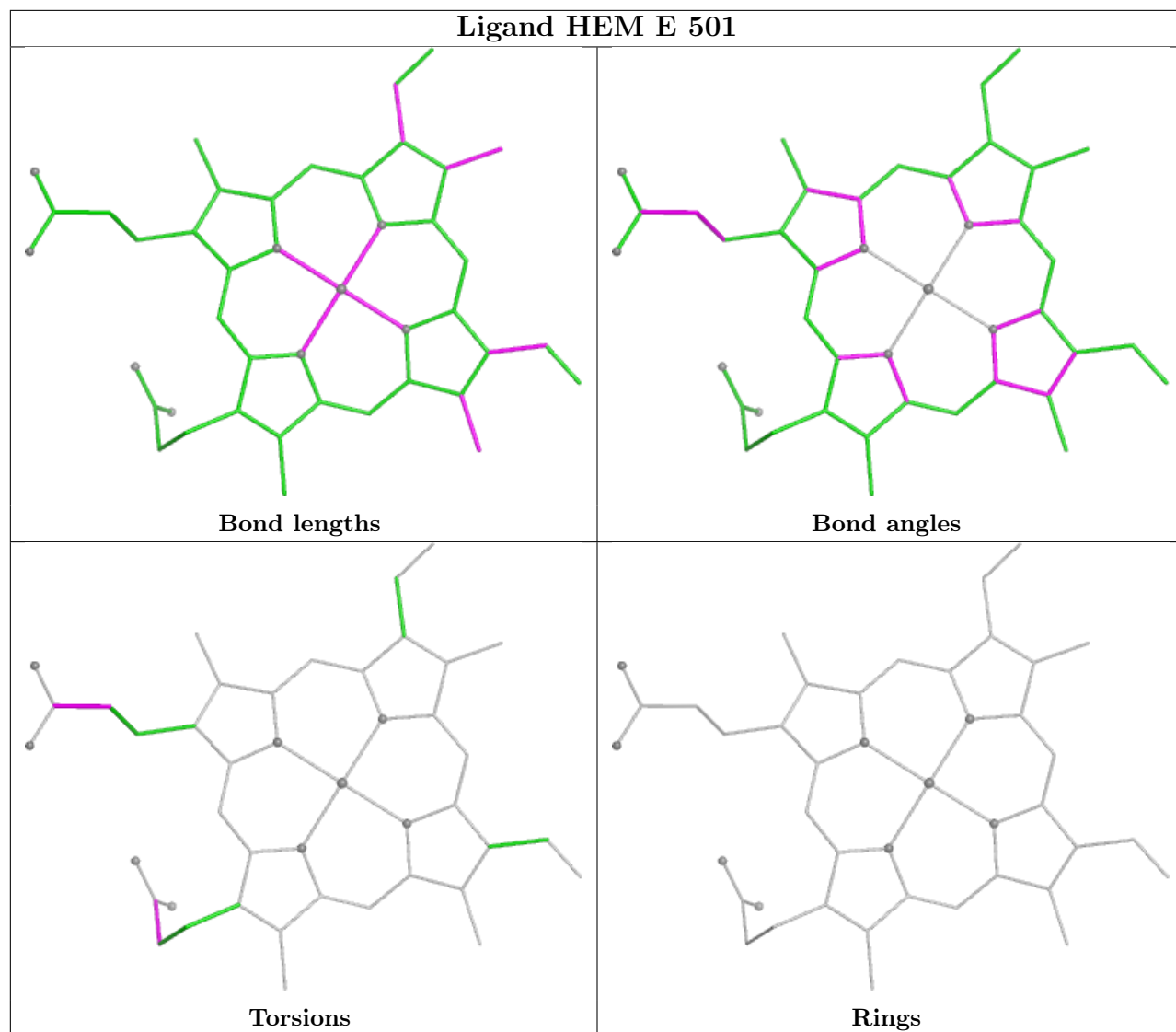
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

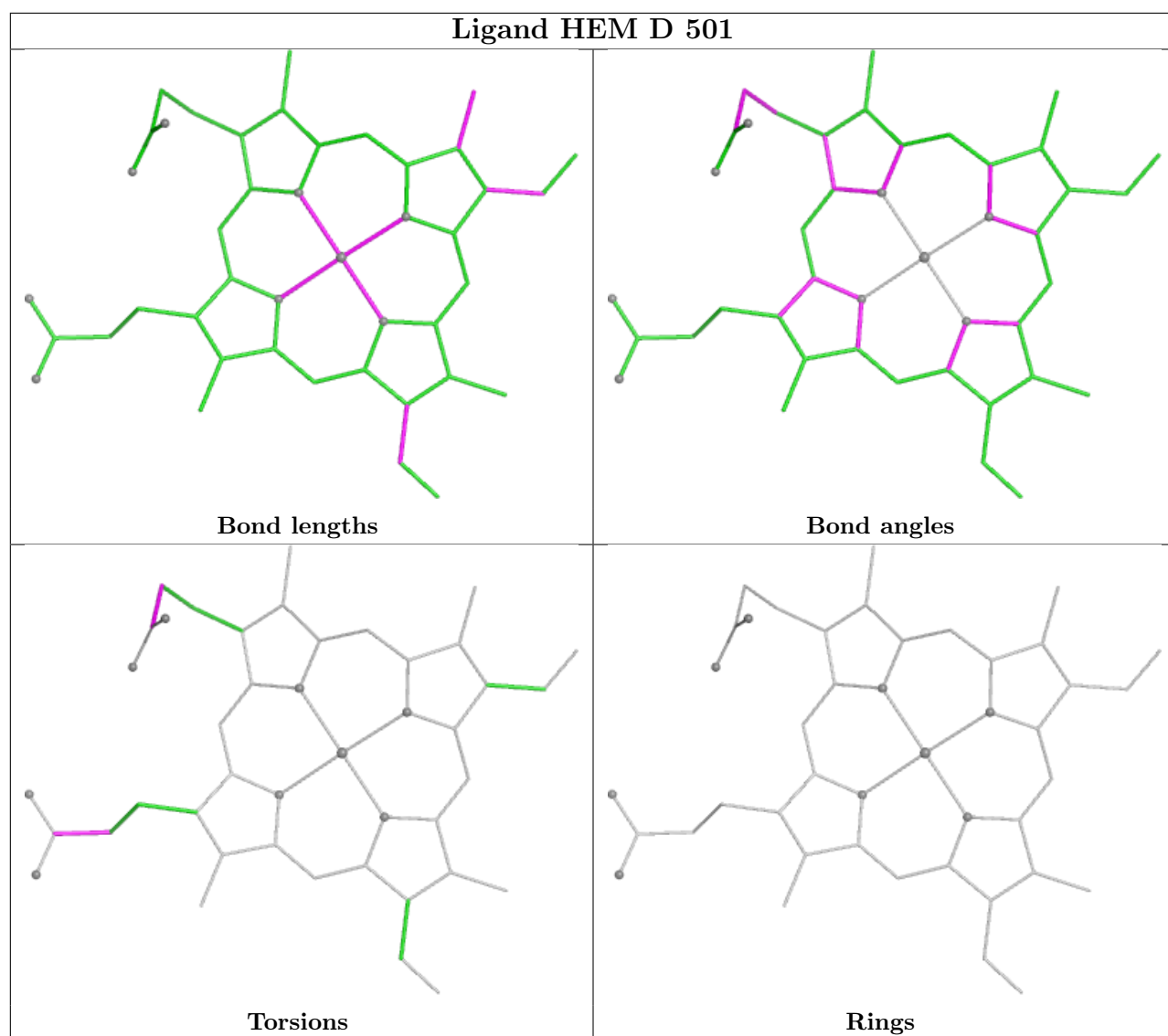












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	354/359 (98%)	-1.14	0 100 100	26, 61, 96, 125	0
1	B	354/359 (98%)	-1.02	1 (0%) 90 89	19, 63, 100, 148	0
1	C	354/359 (98%)	-1.02	0 100 100	34, 65, 101, 120	0
1	D	353/359 (98%)	-0.84	0 100 100	35, 69, 92, 127	0
1	E	354/359 (98%)	-0.74	0 100 100	50, 75, 101, 138	0
1	F	354/359 (98%)	-0.87	0 100 100	46, 82, 107, 135	0
All	All	2123/2154 (98%)	-0.94	1 (0%) 100 100	19, 70, 102, 148	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	242	THR	2.7

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](#)

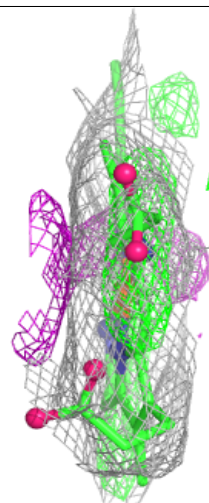
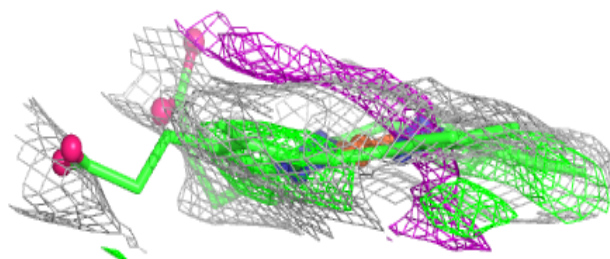
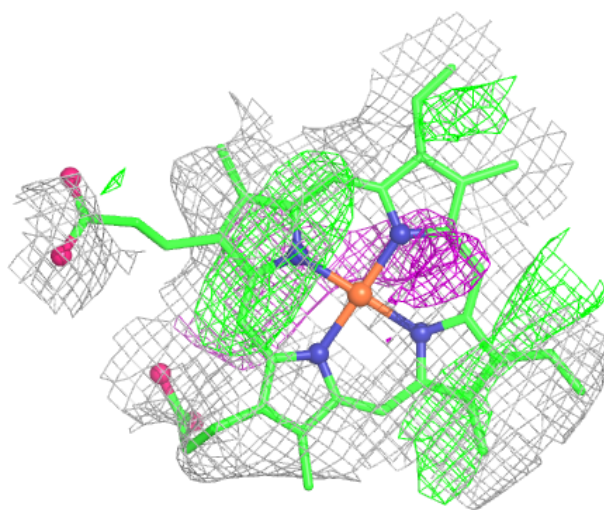
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	HEM	F	501	43/43	0.98	0.09	56,101,118,125	0
2	HEM	B	501	43/43	0.99	0.05	32,56,97,119	0
2	HEM	C	501	43/43	0.99	0.06	61,77,101,113	0
2	HEM	D	501	43/43	0.99	0.05	32,65,80,88	0
2	HEM	E	501	43/43	0.99	0.03	23,41,79,95	0
2	HEM	A	501	43/43	0.99	0.05	26,60,72,79	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.

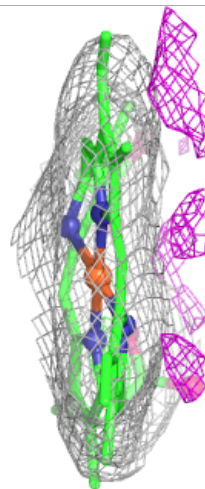
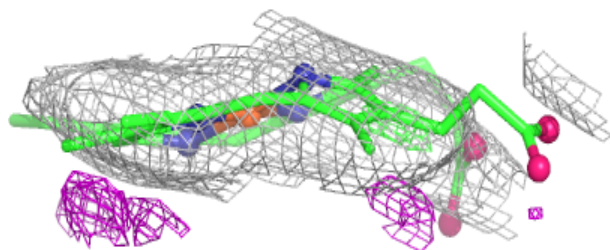
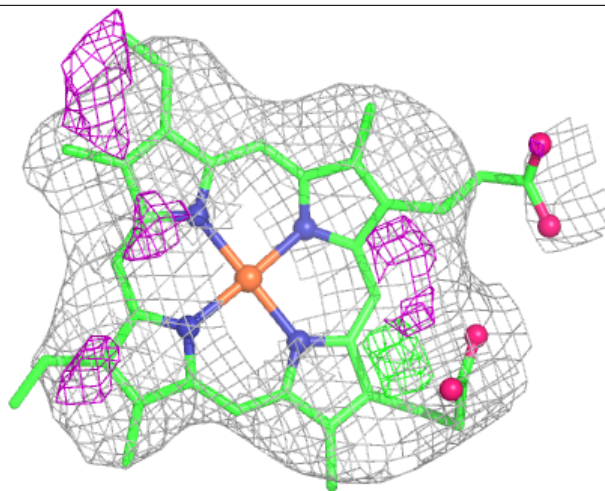
Electron density around HEM F 501:

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



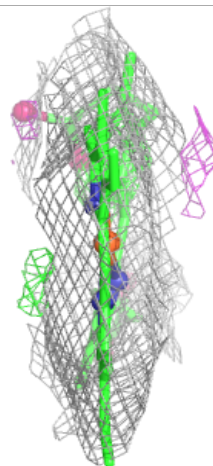
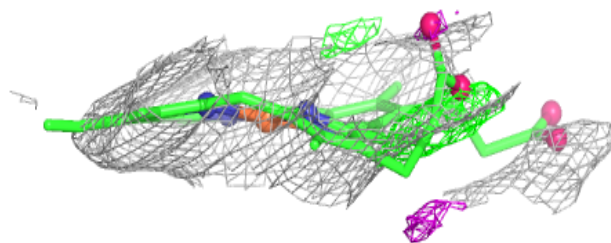
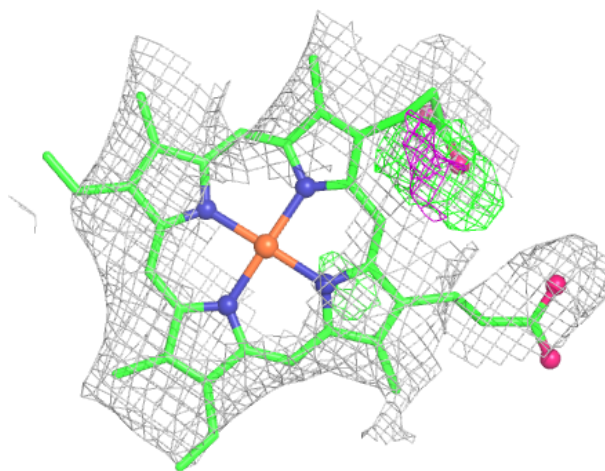
Electron density around HEM B 501:

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



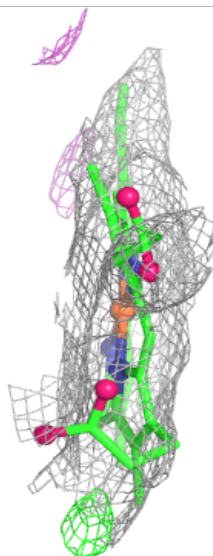
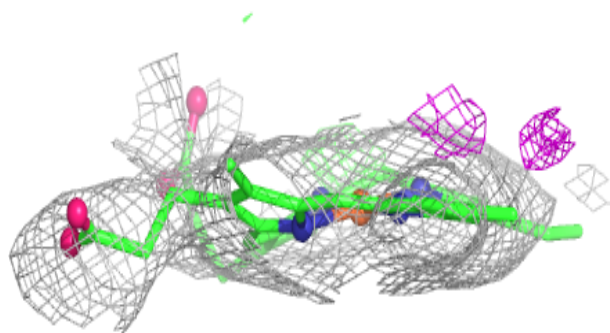
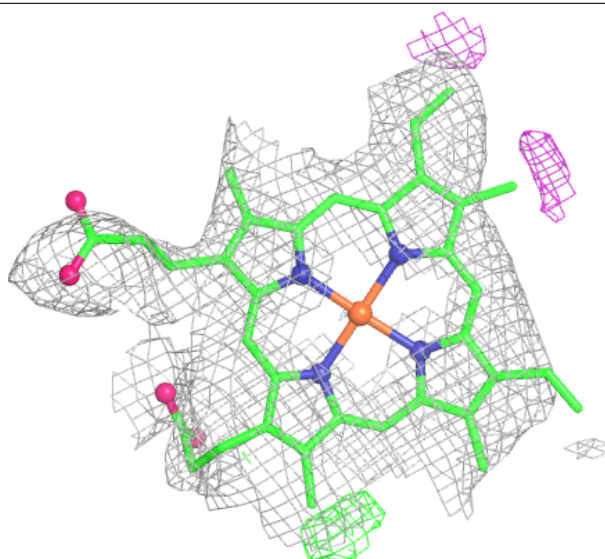
Electron density around HEM C 501:

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



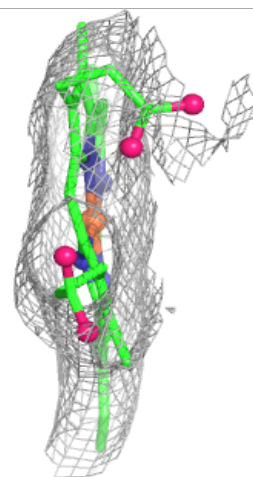
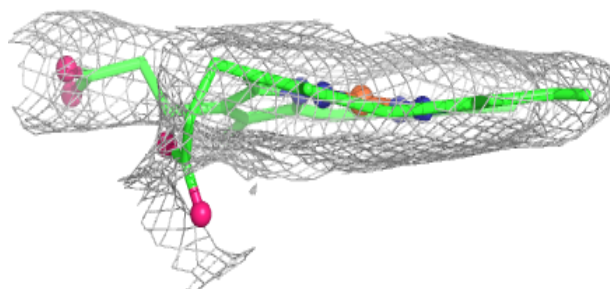
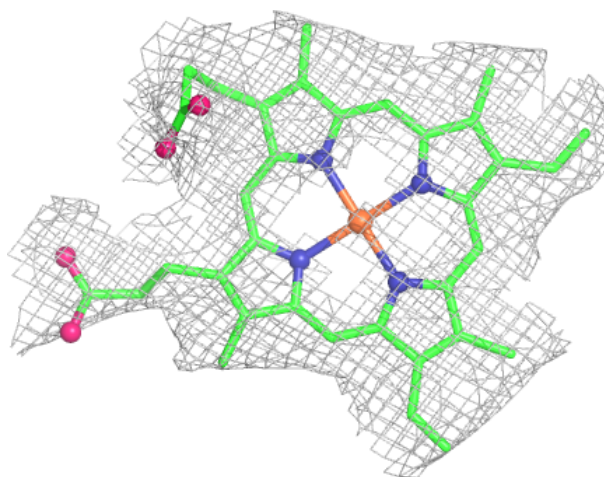
Electron density around HEM D 501:

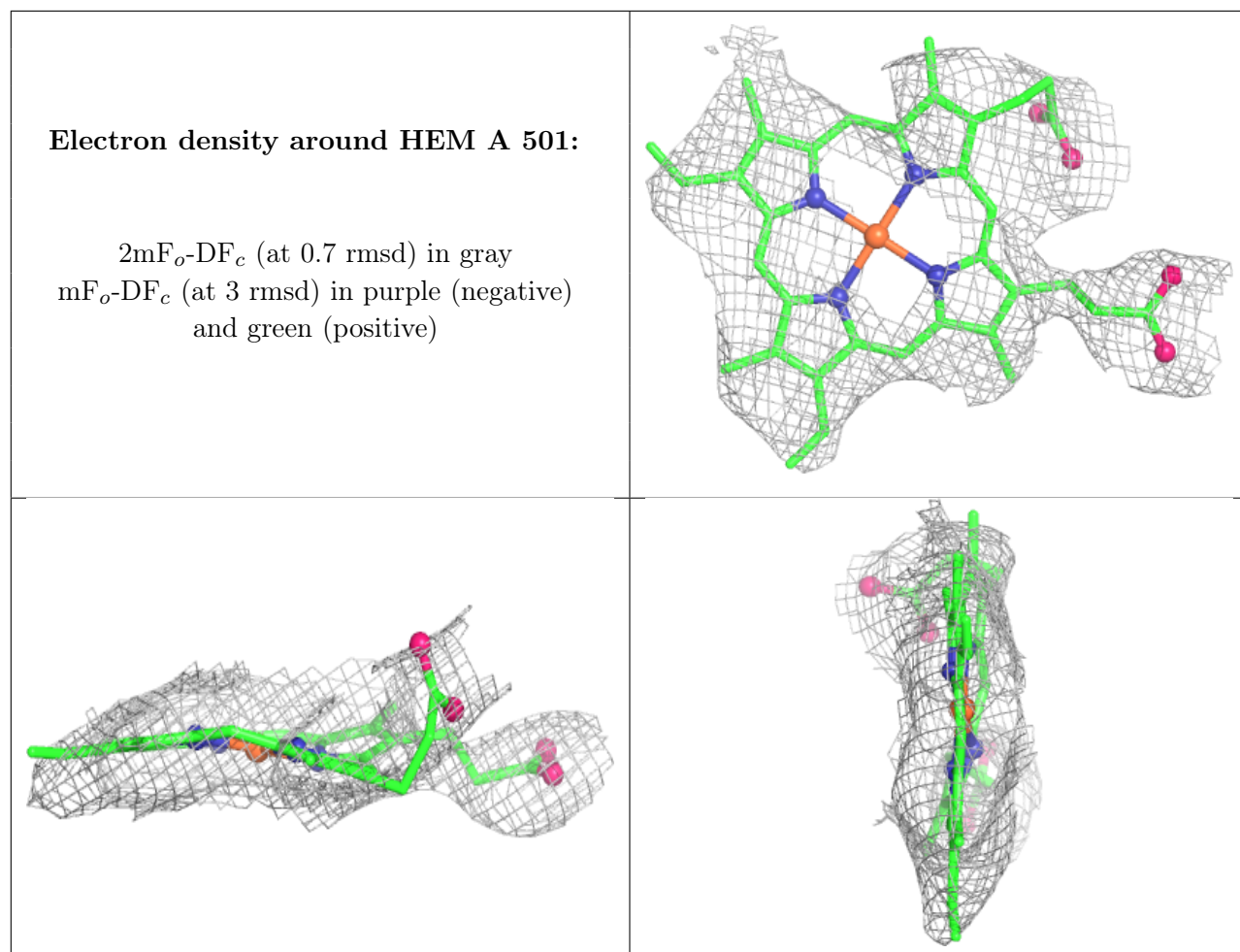
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM E 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.