Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2023 – 07:24 PM EDT

PDB ID	:	8FF7
Title	:	Cytosolic ascorbate peroxidase mutant from Panicum virgatum- ascorbate complex
Authors	:	Zhang, B.; Kang, C.
Deposited on	:	2022-12-07
Resolution	:	2.19 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

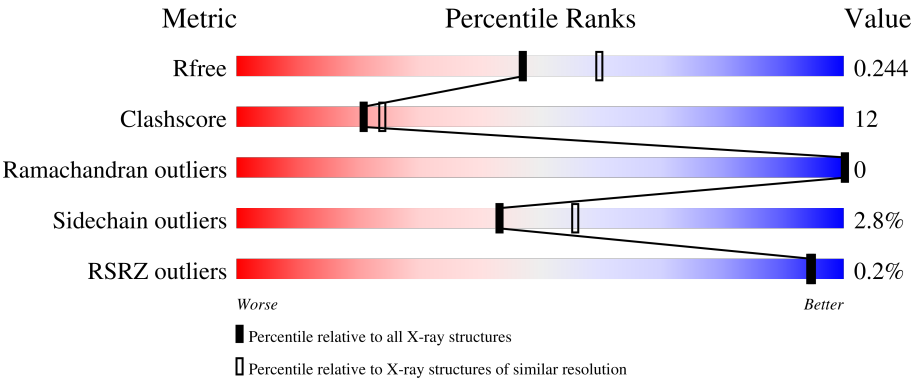
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	80% 19% .
1	B	250	76% 23% .
1	C	250	79% 21%
1	D	250	83% 16% .
1	E	250	74% 26% .

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Mol	Chain	Length	Quality of chain
1	F	250	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13011 atoms, of which 228 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 Cytosolic ascorbate peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1923	1219	331	367	6			
1	B	250	Total	C	N	O	S	0	0	0
			1923	1219	331	367	6			
1	C	250	Total	C	N	O	S	0	0	0
			1923	1219	331	367	6			
1	D	250	Total	C	N	O	S	0	0	0
			1923	1219	331	367	6			
1	E	250	Total	C	N	O	S	0	0	0
			1923	1219	331	367	6			
1	F	250	Total	C	N	O	S	0	0	0
			1923	1219	331	367	6			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	SER	CYS	engineered mutation	UNP A0A8T0NWI5
A	14	ASP	GLU	engineered mutation	UNP A0A8T0NWI5
A	168	ALA	CYS	engineered mutation	UNP A0A8T0NWI5
A	221	ALA	VAL	engineered mutation	UNP A0A8T0NWI5
A	229	ASP	LYS	engineered mutation	UNP A0A8T0NWI5
B	4	SER	CYS	engineered mutation	UNP A0A8T0NWI5
B	14	ASP	GLU	engineered mutation	UNP A0A8T0NWI5
B	168	ALA	CYS	engineered mutation	UNP A0A8T0NWI5
B	221	ALA	VAL	engineered mutation	UNP A0A8T0NWI5
B	229	ASP	LYS	engineered mutation	UNP A0A8T0NWI5
C	4	SER	CYS	engineered mutation	UNP A0A8T0NWI5
C	14	ASP	GLU	engineered mutation	UNP A0A8T0NWI5
C	168	ALA	CYS	engineered mutation	UNP A0A8T0NWI5
C	221	ALA	VAL	engineered mutation	UNP A0A8T0NWI5
C	229	ASP	LYS	engineered mutation	UNP A0A8T0NWI5
D	4	SER	CYS	engineered mutation	UNP A0A8T0NWI5
D	14	ASP	GLU	engineered mutation	UNP A0A8T0NWI5

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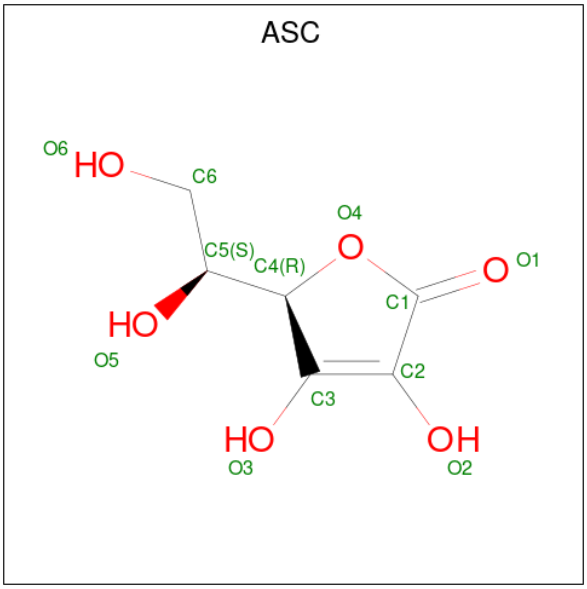
Chain	Residue	Modelled	Actual	Comment	Reference
D	168	ALA	CYS	engineered mutation	UNP A0A8T0NWI5
D	221	ALA	VAL	engineered mutation	UNP A0A8T0NWI5
D	229	ASP	LYS	engineered mutation	UNP A0A8T0NWI5
E	4	SER	CYS	engineered mutation	UNP A0A8T0NWI5
E	14	ASP	GLU	engineered mutation	UNP A0A8T0NWI5
E	168	ALA	CYS	engineered mutation	UNP A0A8T0NWI5
E	221	ALA	VAL	engineered mutation	UNP A0A8T0NWI5
E	229	ASP	LYS	engineered mutation	UNP A0A8T0NWI5
F	4	SER	CYS	engineered mutation	UNP A0A8T0NWI5
F	14	ASP	GLU	engineered mutation	UNP A0A8T0NWI5
F	168	ALA	CYS	engineered mutation	UNP A0A8T0NWI5
F	221	ALA	VAL	engineered mutation	UNP A0A8T0NWI5
F	229	ASP	LYS	engineered mutation	UNP A0A8T0NWI5

- Molecule 2 is ASCORBIC ACID (three-letter code: ASC) (formula: $C_6H_8O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H O 20 6 8 6	0	0
2	B	1	Total C H O 20 6 8 6	0	0
2	C	1	Total C H O 20 6 8 6	0	0
2	D	1	Total C H O 20 6 8 6	0	0
2	E	1	Total C H O 20 6 8 6	0	0

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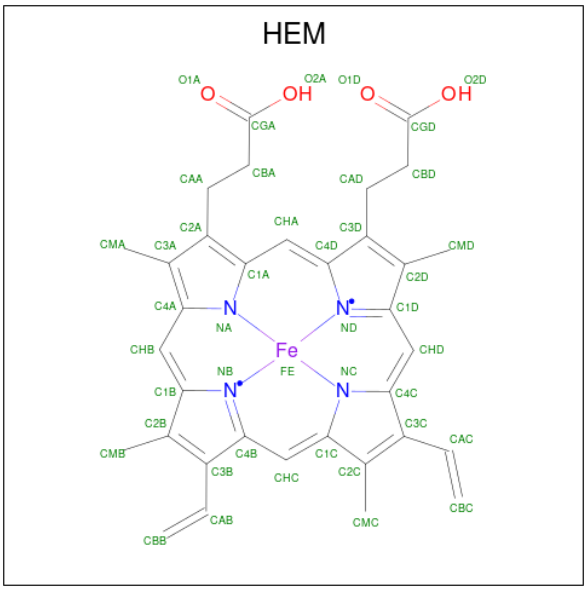
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	F	1	Total	C	H	O	0	0
			20	6	8	6		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Na 1 1	0	0
4	C	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	0	0
4	E	1	Total Na 1 1	0	0
4	F	1	Total Na 1 1	0	0

- Molecule 5 is water.

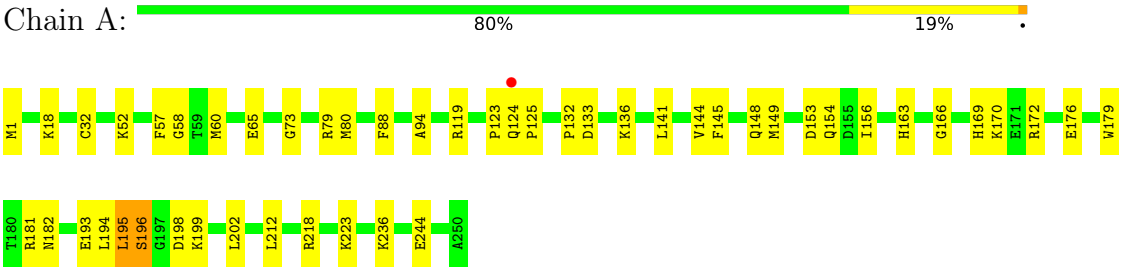
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	181	Total O 181 181	0	0
5	B	146	Total O 146 146	0	0
5	C	145	Total O 145 145	0	0
5	D	178	Total O 178 178	0	0
5	E	135	Total O 135 135	0	0
5	F	124	Total O 124 124	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

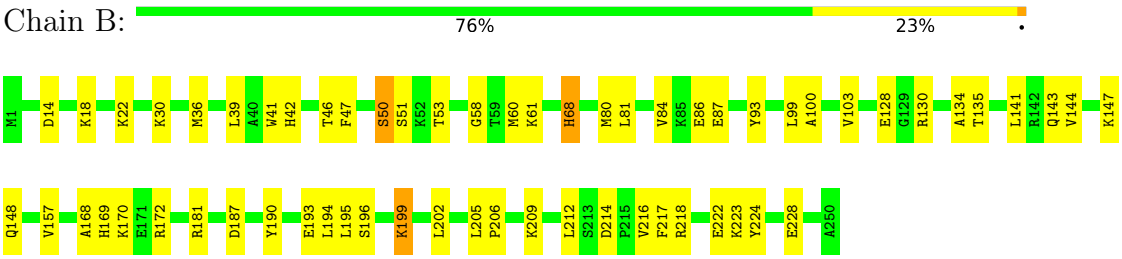
• Molecule 1: Cytosolic ascorbate peroxidase

Chain A:



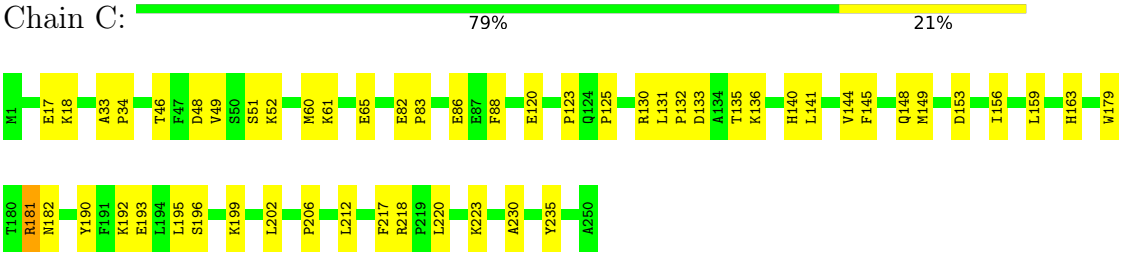
• Molecule 1: Cytosolic ascorbate peroxidase

Chain B:



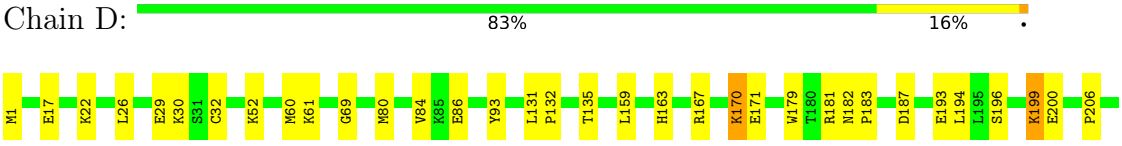
• Molecule 1: Cytosolic ascorbate peroxidase

Chain C:

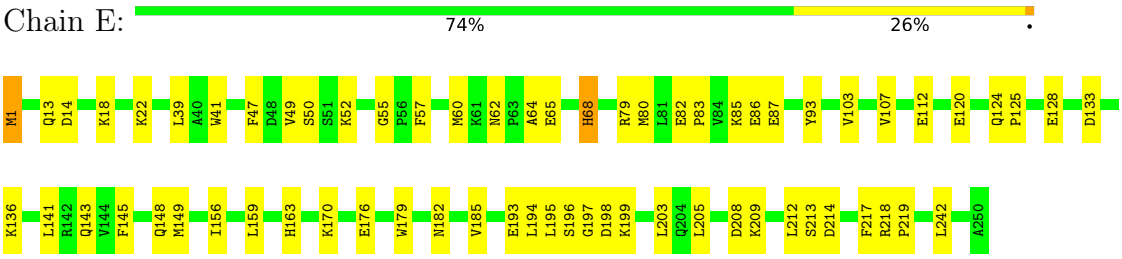


• Molecule 1: Cytosolic ascorbate peroxidase

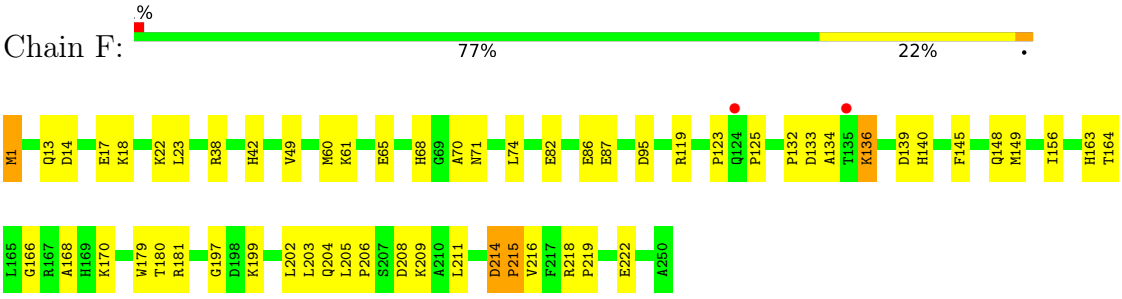
Chain D:



• Molecule 1: Cytosolic ascorbate peroxidase



• Molecule 1: Cytosolic ascorbate peroxidase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	78.27Å 80.18Å 80.17Å 104.55° 101.97° 110.73°	Depositor
Resolution (Å)	49.23 – 2.19 49.23 – 2.19	Depositor EDS
% Data completeness (in resolution range)	97.2 (49.23-2.19) 97.2 (49.23-2.19)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.20	Depositor
R, R_{free}	0.188 , 0.242 0.188 , 0.244	Depositor DCC
R_{free} test set	1993 reflections (2.40%)	wwPDB-VP
Wilson B-factor (Å^2)	28.3	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 34.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13011	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ASC, NA, 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	0.46	0/1971	0.61	0/2668
1	B	0.44	0/1971	0.59	0/2668
1	C	0.43	0/1971	0.57	0/2668
1	D	0.44	0/1971	0.60	0/2668
1	E	0.41	0/1971	0.58	0/2668
1	F	0.41	0/1971	0.59	0/2668
All	All	0.43	0/11826	0.59	0/16008

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1923	0	1884	42	0
1	B	1923	0	1884	61	0
1	C	1923	0	1884	35	0
1	D	1923	0	1885	35	0
1	E	1923	0	1884	53	0
1	F	1923	0	1885	51	0
2	A	12	8	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	12	8	8	0	0
2	C	12	8	8	0	0
2	D	12	8	8	1	0
2	E	12	8	8	0	0
2	F	12	8	8	0	0
3	A	43	30	30	6	0
3	B	43	30	30	6	0
3	C	43	30	30	4	0
3	D	43	30	30	3	0
3	E	43	30	30	5	0
3	F	43	30	30	7	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	181	0	0	5	0
5	B	146	0	0	6	0
5	C	145	0	0	5	0
5	D	178	0	0	9	0
5	E	135	0	0	5	0
5	F	124	0	0	6	0
All	All	12783	228	11534	285	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 12.

All (285) 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:194:LEU:HD12	1:B:212:LEU:HD21	1.32	1.10
1:F:206:PRO:HA	1:F:209:LYS:HD2	1.33	1.06
1:A:145:PHE:HA	1:A:149:MET:HE3	1.38	1.04
1:F:1:MET:N	5:F:401:HOH:O	2.01	0.93
1:D:170:LYS:NZ	5:D:401:HOH:O	2.02	0.91
1:F:203:LEU:HD11	1:F:205:LEU:HD23	1.53	0.88
1:E:1:MET:SD	1:E:1:MET:N	2.46	0.87
1:E:83:PRO:HA	1:E:86:GLU:HG3	1.56	0.87
1:E:143:GLN:O	1:E:148:GLN:HG3	1.76	0.85
1:B:194:LEU:HD12	1:B:212:LEU:CD2	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:GLN:NE2	5:E:403:HOH:O	2.11	0.83
1:F:197:GLY:O	1:F:199:LYS:NZ	2.15	0.80
1:D:200:GLU:N	1:D:200:GLU:OE1	2.15	0.79
1:E:1:MET:N	5:E:404:HOH:O	2.15	0.78
1:B:218:ARG:HD2	1:B:222:GLU:OE2	1.83	0.78
1:B:199:LYS:NZ	5:B:402:HOH:O	2.16	0.78
1:B:193:GLU:OE1	1:B:199:LYS:HE2	1.85	0.76
1:E:141:LEU:HD22	3:E:302:HEM:HBB1	1.66	0.76
1:F:133:ASP:OD2	1:F:136:LYS:HD2	1.84	0.76
1:A:132:PRO:HD3	1:A:144:VAL:HG11	1.69	0.75
1:B:36:MET:HE3	1:B:36:MET:HA	1.70	0.74
1:B:143:GLN:HE21	1:B:148:GLN:HE21	1.37	0.73
1:C:181:ARG:HD3	5:C:467:HOH:O	1.88	0.73
1:F:208:ASP:O	1:F:211:LEU:HB2	1.87	0.73
1:B:222:GLU:OE1	5:B:401:HOH:O	2.06	0.72
1:F:203:LEU:HD12	1:F:204:GLN:H	1.54	0.72
1:E:182:ASN:ND2	1:E:185:VAL:HB	2.05	0.72
1:B:36:MET:HE1	1:B:81:LEU:HD11	1.72	0.72
1:F:203:LEU:HD12	1:F:204:GLN:N	2.05	0.71
1:A:195:LEU:HD13	1:A:212:LEU:HD22	1.73	0.71
1:D:218:ARG:HB3	1:D:219:PRO:HD3	1.73	0.71
1:E:195:LEU:HD13	1:E:212:LEU:CD2	2.21	0.71
1:F:204:GLN:NE2	5:F:402:HOH:O	2.18	0.70
1:E:22:LYS:HE3	1:E:87:GLU:OE1	1.92	0.70
1:D:29:GLU:OE2	5:D:403:HOH:O	2.10	0.70
1:B:22:LYS:HD3	1:B:84:VAL:HG22	1.74	0.70
1:E:49:VAL:O	1:E:52:LYS:HD3	1.91	0.69
1:E:213:SER:OG	5:E:401:HOH:O	2.08	0.69
1:E:218:ARG:HB3	1:E:219:PRO:HD3	1.74	0.69
1:D:200:GLU:O	5:D:402:HOH:O	2.10	0.69
1:F:82:GLU:O	1:F:86:GLU:HG2	1.92	0.68
1:D:171:GLU:OE1	1:D:171:GLU:N	2.15	0.68
1:C:17:GLU:OE1	5:C:401:HOH:O	2.12	0.68
1:C:60:MET:HG3	1:C:60:MET:O	1.93	0.68
1:A:181:ARG:HD3	1:A:202:LEU:HD21	1.76	0.67
3:C:302:HEM:HMB2	3:C:302:HEM:HBB2	1.76	0.67
1:E:198:ASP:OD2	1:E:209:LYS:NZ	2.27	0.67
1:B:22:LYS:CD	1:B:84:VAL:HG22	2.26	0.66
1:E:120:GLU:HA	1:E:120:GLU:OE1	1.95	0.66
1:B:36:MET:CE	1:B:81:LEU:HD11	2.27	0.65
1:F:38:ARG:NH2	1:F:70:ALA:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:65:GLU:HA	1:F:68:HIS:CE1	2.32	0.64
1:A:80:MET:HE3	5:C:523:HOH:O	1.97	0.64
1:B:60:MET:O	1:B:60:MET:HG3	1.98	0.64
1:D:170:LYS:HE3	5:D:494:HOH:O	1.99	0.63
3:E:302:HEM:HMB2	3:E:302:HEM:HBB2	1.80	0.63
1:F:60:MET:O	1:F:60:MET:HG3	1.96	0.63
1:E:124:GLN:HG2	5:E:519:HOH:O	1.99	0.63
1:A:218:ARG:HG2	5:A:544:HOH:O	1.98	0.62
1:E:112:GLU:HG3	5:E:421:HOH:O	1.97	0.62
1:B:212:LEU:HD22	1:B:212:LEU:H	1.64	0.62
1:C:82:GLU:O	1:C:86:GLU:HG2	1.99	0.61
1:C:135:THR:HA	1:C:206:PRO:HG2	1.82	0.61
1:E:14:ASP:OD2	1:E:18:LYS:HE2	2.00	0.60
1:D:30:LYS:HD2	1:D:80:MET:CE	2.31	0.60
1:C:141:LEU:HD22	3:C:302:HEM:HBB1	1.82	0.60
1:E:195:LEU:HD13	1:E:212:LEU:HD22	1.83	0.60
1:C:145:PHE:HA	1:C:149:MET:HE3	1.82	0.60
1:F:14:ASP:OD2	1:F:18:LYS:HE2	2.02	0.59
1:B:50:SER:HB2	5:B:446:HOH:O	2.02	0.59
1:F:123:PRO:O	1:F:125:PRO:HD3	2.02	0.59
1:A:170:LYS:HB2	1:A:176:GLU:OE1	2.02	0.59
1:A:198:ASP:O	5:A:401:HOH:O	2.17	0.59
1:F:133:ASP:HB3	1:F:136:LYS:HD2	1.85	0.59
1:C:61:LYS:NZ	1:C:82:GLU:OE1	2.35	0.59
1:F:202:LEU:HD12	5:F:502:HOH:O	2.01	0.59
1:C:48:ASP:OD2	1:C:51:SER:OG	2.14	0.58
1:D:163:HIS:HB3	1:D:179:TRP:CD2	2.37	0.58
1:C:144:VAL:O	1:C:148:GLN:HB2	2.03	0.58
1:E:60:MET:SD	1:E:65:GLU:HG2	2.45	0.57
1:B:212:LEU:HD22	1:B:212:LEU:N	2.20	0.57
1:A:181:ARG:HG3	1:E:64:ALA:HA	1.87	0.57
1:B:22:LYS:HE2	1:B:87:GLU:OE1	2.05	0.57
1:B:143:GLN:NE2	1:B:148:GLN:HE21	2.02	0.57
1:A:195:LEU:HD13	1:A:212:LEU:CD2	2.33	0.56
1:A:141:LEU:HD22	3:A:302:HEM:HBB1	1.87	0.56
1:F:166:GLY:HA3	3:F:302:HEM:HAD1	1.86	0.56
3:B:302:HEM:HBB2	3:B:302:HEM:HMB2	1.86	0.56
1:A:145:PHE:CA	1:A:149:MET:HE3	2.27	0.55
1:B:46:THR:O	1:B:130:ARG:HD2	2.08	0.54
1:B:144:VAL:O	1:B:148:GLN:HB2	2.07	0.54
1:E:82:GLU:O	1:E:86:GLU:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ASN:N	1:A:182:ASN:OD1	2.40	0.54
1:F:134:ALA:HB1	1:F:205:LEU:HD13	1.89	0.54
1:D:212:LEU:O	1:D:218:ARG:NH1	2.40	0.54
1:F:179:TRP:O	1:F:202:LEU:HD13	2.07	0.54
1:F:214:ASP:OD1	1:F:216:VAL:N	2.41	0.53
1:D:60:MET:O	1:D:60:MET:HG3	2.07	0.53
1:D:30:LYS:HD2	1:D:80:MET:HE2	1.91	0.53
1:A:212:LEU:O	1:A:218:ARG:HD2	2.09	0.53
1:F:204:GLN:HG3	5:F:402:HOH:O	2.08	0.53
1:A:144:VAL:O	1:A:148:GLN:HB2	2.09	0.52
1:B:36:MET:HE1	1:B:81:LEU:CD1	2.39	0.52
1:D:187:ASP:HB2	1:D:228:GLU:OE2	2.08	0.52
1:A:60:MET:HG3	1:A:60:MET:O	2.10	0.52
1:C:190:TYR:HB3	5:C:483:HOH:O	2.10	0.52
1:F:148:GLN:NE2	5:F:403:HOH:O	2.23	0.52
1:B:141:LEU:HD22	3:B:302:HEM:HBB1	1.91	0.52
1:A:124:GLN:HA	1:A:124:GLN:OE1	2.09	0.52
1:D:22:LYS:HG2	1:D:84:VAL:HG22	1.91	0.51
1:D:131:LEU:HB3	1:D:132:PRO:HD2	1.91	0.51
1:F:49:VAL:HG12	1:F:148:GLN:O	2.10	0.51
1:E:65:GLU:HA	1:E:68:HIS:CE1	2.45	0.51
1:D:52:LYS:NZ	5:D:410:HOH:O	2.43	0.51
3:F:302:HEM:HBB2	3:F:302:HEM:HHC	1.91	0.51
1:F:134:ALA:HA	3:F:302:HEM:CMB	2.40	0.51
1:E:62:ASN:HD22	1:E:125:PRO:CG	2.23	0.51
1:F:168:ALA:HA	3:F:302:HEM:HAA1	1.92	0.51
1:B:36:MET:CE	1:B:39:LEU:HD23	2.40	0.51
1:B:61:LYS:NZ	1:B:93:TYR:OH	2.44	0.51
1:B:68:HIS:CE1	1:B:128:GLU:HB2	2.46	0.51
1:F:22:LYS:HE2	5:F:517:HOH:O	2.09	0.51
1:E:83:PRO:CA	1:E:86:GLU:HG3	2.37	0.50
1:C:195:LEU:HD23	1:C:212:LEU:HD22	1.92	0.50
1:A:73:GLY:HA3	1:A:172:ARG:HD3	1.93	0.50
1:C:181:ARG:HG2	5:C:476:HOH:O	2.12	0.50
1:D:159:LEU:HB3	3:D:302:HEM:HMC3	1.94	0.50
1:B:135:THR:HA	1:B:206:PRO:HG2	1.94	0.50
1:A:133:ASP:OD2	1:A:136:LYS:NZ	2.45	0.50
1:B:196:SER:HB3	1:B:199:LYS:HE3	1.93	0.50
1:B:36:MET:HA	1:B:36:MET:CE	2.41	0.49
1:B:51:SER:HB2	1:B:53:THR:HG23	1.94	0.49
3:A:302:HEM:HBB2	3:A:302:HEM:HMB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:GLU:OE1	1:E:199:LYS:NZ	2.37	0.49
1:E:163:HIS:HB3	1:E:179:TRP:CD2	2.47	0.49
1:A:79:ARG:NE	5:A:406:HOH:O	2.41	0.49
1:A:123:PRO:O	1:A:125:PRO:HD3	2.12	0.49
1:B:168:ALA:HA	3:B:302:HEM:O2A	2.13	0.49
1:F:134:ALA:O	1:F:206:PRO:HD2	2.13	0.49
1:A:163:HIS:HB3	1:A:179:TRP:CD2	2.48	0.48
1:A:169:HIS:HB2	1:A:172:ARG:HG3	1.95	0.48
1:F:181:ARG:NH2	1:F:202:LEU:HG	2.28	0.48
1:D:135:THR:HA	1:D:206:PRO:HG2	1.95	0.48
1:B:157:VAL:HG12	1:B:224:TYR:CE2	2.49	0.48
1:E:197:GLY:O	1:E:199:LYS:HE3	2.13	0.48
1:B:143:GLN:O	1:B:148:GLN:HG3	2.13	0.48
1:A:18:LYS:HB3	1:A:88:PHE:CZ	2.49	0.47
1:C:18:LYS:HB3	1:C:88:PHE:CE1	2.50	0.47
1:B:187:ASP:HB2	1:B:228:GLU:OE2	2.15	0.47
1:A:57:PHE:C	1:A:94:ALA:HB2	2.34	0.47
1:F:145:PHE:HB2	1:F:156:ILE:HD11	1.96	0.47
1:C:153:ASP:HA	1:C:156:ILE:HD12	1.96	0.47
1:C:46:THR:O	1:C:130:ARG:HD2	2.14	0.47
1:E:133:ASP:HB3	1:E:136:LYS:HD3	1.96	0.47
1:A:58:GLY:N	1:A:94:ALA:HB2	2.30	0.47
1:B:36:MET:HE1	1:B:39:LEU:HD23	1.95	0.47
1:B:42:HIS:NE2	5:B:407:HOH:O	2.36	0.47
1:B:195:LEU:HD23	1:B:212:LEU:HD12	1.97	0.47
1:E:41:TRP:HE3	1:E:242:LEU:HD21	1.80	0.47
1:F:61:LYS:O	1:F:61:LYS:HG3	2.14	0.47
1:A:181:ARG:HG3	1:E:64:ALA:CB	2.45	0.47
1:C:199:LYS:HD2	1:C:202:LEU:HD12	1.96	0.46
1:D:61:LYS:HD3	1:D:93:TYR:CZ	2.51	0.46
1:B:157:VAL:HG12	1:B:224:TYR:HE2	1.80	0.46
1:B:190:TYR:HB3	5:B:432:HOH:O	2.14	0.46
1:E:55:GLY:O	1:E:57:PHE:N	2.48	0.46
1:B:86:GLU:CD	1:E:79:ARG:HE	2.19	0.46
1:C:223:LYS:HE3	1:C:230:ALA:HB1	1.98	0.46
1:A:154:GLN:HG2	5:A:474:HOH:O	2.16	0.45
1:B:212:LEU:CD2	1:B:212:LEU:H	2.28	0.45
3:C:302:HEM:HBB2	3:C:302:HEM:CMB	2.46	0.45
1:E:170:LYS:HB2	1:E:176:GLU:CG	2.46	0.45
1:C:83:PRO:HA	1:C:86:GLU:HG3	1.97	0.45
1:D:52:LYS:NZ	5:D:406:HOH:O	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:GLU:O	1:D:86:GLU:HG3	2.16	0.45
3:F:302:HEM:HBC2	3:F:302:HEM:HMC1	1.99	0.45
1:A:195:LEU:CD1	1:A:212:LEU:HD22	2.44	0.45
1:E:49:VAL:HG12	1:E:148:GLN:O	2.15	0.45
3:E:302:HEM:HBB2	3:E:302:HEM:CMB	2.46	0.45
1:A:141:LEU:CD2	3:A:302:HEM:HBB1	2.46	0.45
1:D:61:LYS:HD3	1:D:93:TYR:CE1	2.52	0.45
1:D:193:GLU:OE1	1:D:199:LYS:NZ	2.47	0.45
1:B:134:ALA:HB1	1:B:205:LEU:HD13	1.98	0.45
1:C:18:LYS:HB3	1:C:88:PHE:CZ	2.51	0.45
1:F:134:ALA:HA	3:F:302:HEM:HMB1	1.98	0.45
1:D:194:LEU:O	1:D:212:LEU:HD11	2.16	0.45
1:F:218:ARG:O	1:F:222:GLU:HG3	2.17	0.45
1:C:123:PRO:O	1:C:125:PRO:HD3	2.17	0.45
1:E:159:LEU:HB3	3:E:302:HEM:HMC3	1.99	0.45
1:C:131:LEU:HB3	1:C:132:PRO:HD2	1.98	0.45
1:E:194:LEU:HD21	1:E:208:ASP:HB3	1.99	0.45
1:F:209:LYS:C	1:F:211:LEU:N	2.71	0.45
1:B:195:LEU:HD23	1:B:212:LEU:CD1	2.47	0.44
3:B:302:HEM:HBB2	3:B:302:HEM:CMB	2.47	0.44
1:E:68:HIS:CD2	1:E:128:GLU:HB2	2.51	0.44
1:E:103:VAL:O	1:E:107:VAL:HG22	2.17	0.44
1:E:145:PHE:CB	1:E:156:ILE:HG12	2.46	0.44
1:B:22:LYS:HD2	1:B:84:VAL:HG22	1.99	0.44
1:B:53:THR:OG1	1:B:130:ARG:NH2	2.48	0.44
1:F:23:LEU:HD23	1:F:23:LEU:HA	1.78	0.44
1:F:181:ARG:NE	1:F:202:LEU:HD21	2.32	0.44
1:B:14:ASP:OD2	1:B:18:LYS:HE3	2.18	0.44
3:B:302:HEM:HBA2	3:B:302:HEM:HHA	1.99	0.44
1:E:60:MET:HA	1:E:65:GLU:HG2	1.99	0.44
1:E:196:SER:CB	1:E:199:LYS:HE2	2.48	0.44
1:F:13:GLN:OE1	1:F:17:GLU:HG2	2.17	0.44
1:F:42:HIS:ND1	1:F:71:ASN:OD1	2.45	0.44
1:F:95:ASP:OD1	1:F:119:ARG:HB2	2.17	0.44
1:C:181:ARG:HH11	1:C:202:LEU:HD11	1.83	0.44
1:D:32:CYS:HA	2:D:301:ASC:O4	2.17	0.44
1:F:181:ARG:HH21	1:F:199:LYS:HD2	1.83	0.44
3:F:302:HEM:HBC2	3:F:302:HEM:CMC	2.48	0.44
1:C:133:ASP:H	1:C:140:HIS:CD2	2.36	0.43
1:B:181:ARG:HD3	1:B:202:LEU:HD21	2.00	0.43
1:C:33:ALA:HB3	1:C:34:PRO:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:215:PRO:O	1:F:219:PRO:CD	2.66	0.43
1:F:133:ASP:CB	1:F:136:LYS:HD2	2.47	0.43
1:F:203:LEU:HD11	1:F:205:LEU:CD2	2.36	0.43
1:B:214:ASP:HB3	1:B:217:PHE:HB2	2.00	0.43
1:A:169:HIS:ND1	3:A:302:HEM:O1A	2.28	0.43
1:B:58:GLY:HA2	5:B:503:HOH:O	2.19	0.43
1:E:47:PHE:CE2	1:E:49:VAL:HA	2.52	0.43
1:D:181:ARG:NH2	5:D:402:HOH:O	2.16	0.43
1:A:236:LYS:HD2	5:A:455:HOH:O	2.19	0.43
1:B:134:ALA:CB	1:B:205:LEU:HD13	2.49	0.43
1:B:169:HIS:N	3:B:302:HEM:O2A	2.42	0.43
1:A:18:LYS:HB3	1:A:88:PHE:CE1	2.54	0.42
1:D:69:GLY:O	5:D:404:HOH:O	2.22	0.42
1:E:203:LEU:HD21	1:E:205:LEU:HD21	2.01	0.42
1:E:214:ASP:HB3	1:E:217:PHE:HB2	2.01	0.42
1:A:193:GLU:HA	1:A:193:GLU:OE1	2.19	0.42
1:B:99:LEU:O	1:B:103:VAL:HG23	2.18	0.42
1:C:235:TYR:CD1	1:C:235:TYR:C	2.93	0.42
1:E:141:LEU:HD22	3:E:302:HEM:CBB	2.43	0.42
1:B:209:LYS:HA	1:B:212:LEU:HD23	2.00	0.42
1:E:39:LEU:HD12	1:E:60:MET:HG2	2.02	0.42
1:A:119:ARG:NH2	1:A:244:GLU:HG2	2.35	0.42
1:D:214:ASP:HB3	1:D:217:PHE:HB2	2.02	0.42
1:A:236:LYS:HB3	1:A:236:LYS:HE2	1.89	0.42
3:A:302:HEM:HBA2	3:A:302:HEM:HHA	2.02	0.42
1:C:133:ASP:HB3	1:C:136:LYS:HG3	2.01	0.42
1:C:182:ASN:N	1:C:182:ASN:OD1	2.53	0.42
1:E:193:GLU:OE1	1:E:193:GLU:HA	2.20	0.42
1:F:163:HIS:HB3	1:F:179:TRP:CD2	2.54	0.42
1:A:153:ASP:HA	1:A:156:ILE:HD12	2.02	0.42
1:C:217:PHE:O	1:C:220:LEU:HB2	2.19	0.42
1:A:196:SER:HB3	1:A:199:LYS:HE2	2.01	0.41
1:D:167:ARG:NH2	1:D:183:PRO:HG3	2.34	0.41
1:B:214:ASP:OD1	1:B:216:VAL:N	2.52	0.41
1:D:224:TYR:CD1	1:D:231:PHE:HA	2.55	0.41
1:E:196:SER:HB2	1:E:199:LYS:HE2	2.01	0.41
1:A:32:CYS:HA	2:A:301:ASC:O4	2.21	0.41
1:B:47:PHE:HA	1:B:53:THR:O	2.20	0.41
1:C:193:GLU:HA	1:C:193:GLU:OE1	2.20	0.41
1:D:224:TYR:HB3	1:D:231:PHE:HB2	2.03	0.41
3:D:302:HEM:HHC	3:D:302:HEM:HBB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:145:PHE:CG	1:E:156:ILE:HG12	2.56	0.41
1:B:68:HIS:CD2	1:B:128:GLU:HB2	2.56	0.41
1:B:86:GLU:OE2	1:E:79:ARG:NE	2.52	0.41
1:C:163:HIS:HB3	1:C:179:TRP:CD2	2.56	0.41
1:B:30:LYS:HD2	1:B:80:MET:CE	2.51	0.41
1:C:159:LEU:HB3	3:C:302:HEM:HMC3	2.03	0.41
1:D:239:HIS:O	1:D:239:HIS:HD2	2.04	0.41
1:B:169:HIS:HB2	1:B:172:ARG:HG3	2.03	0.41
1:A:166:GLY:HA3	3:A:302:HEM:O2D	2.21	0.41
1:B:68:HIS:NE2	1:B:128:GLU:HB2	2.35	0.41
1:B:143:GLN:HE21	1:B:148:GLN:NE2	2.13	0.41
1:C:49:VAL:O	1:C:52:LYS:HD3	2.21	0.41
1:D:159:LEU:HB3	3:D:302:HEM:CMC	2.51	0.41
1:F:22:LYS:HE3	1:F:87:GLU:OE1	2.20	0.41
1:F:74:LEU:HA	1:F:74:LEU:HD23	1.86	0.41
1:F:136:LYS:HB2	1:F:140:HIS:CD2	2.56	0.41
1:F:164:THR:HA	1:F:180:THR:HG21	2.03	0.41
1:F:214:ASP:OD1	1:F:216:VAL:HG22	2.20	0.41
1:D:17:GLU:HG3	5:D:574:HOH:O	2.21	0.41
1:D:26:LEU:C	1:D:26:LEU:HD23	2.41	0.41
1:A:60:MET:SD	1:A:65:GLU:HG2	2.61	0.40
1:C:60:MET:SD	1:C:65:GLU:HG2	2.61	0.40
1:F:215:PRO:O	1:F:219:PRO:HD3	2.21	0.40
1:B:36:MET:HE2	1:B:100:ALA:HB1	2.02	0.40
1:A:181:ARG:HG3	1:E:64:ALA:CA	2.51	0.40
1:C:196:SER:HB2	1:C:199:LYS:CE	2.51	0.40
1:E:85:LYS:HE3	1:E:93:TYR:CE2	2.56	0.40
1:E:145:PHE:HA	1:E:149:MET:HE3	2.04	0.40
1:F:145:PHE:O	1:F:149:MET:HB2	2.20	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	248/250 (99%)	243 (98%)	5 (2%)	0	100	100
1	B	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
1	C	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
1	D	248/250 (99%)	246 (99%)	2 (1%)	0	100	100
1	E	248/250 (99%)	241 (97%)	7 (3%)	0	100	100
1	F	248/250 (99%)	239 (96%)	9 (4%)	0	100	100
All	All	1488/1500 (99%)	1453 (98%)	35 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	200/200 (100%)	194 (97%)	6 (3%)	41	53
1	B	200/200 (100%)	193 (96%)	7 (4%)	36	46
1	C	200/200 (100%)	196 (98%)	4 (2%)	55	69
1	D	200/200 (100%)	195 (98%)	5 (2%)	47	60
1	E	200/200 (100%)	196 (98%)	4 (2%)	55	69
1	F	200/200 (100%)	193 (96%)	7 (4%)	36	46
All	All	1200/1200 (100%)	1167 (97%)	33 (3%)	43	56

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	52	LYS
1	A	194	LEU
1	A	195	LEU
1	A	196	SER
1	A	223	LYS
1	B	41	TRP

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Mol	Chain	Res	Type
1	B	50	SER
1	B	68	HIS
1	B	147	LYS
1	B	170	LYS
1	B	199	LYS
1	B	223	LYS
1	C	120	GLU
1	C	181	ARG
1	C	192	LYS
1	C	218	ARG
1	D	1	MET
1	D	170	LYS
1	D	182	ASN
1	D	196	SER
1	D	199	LYS
1	E	1	MET
1	E	50	SER
1	E	68	HIS
1	E	80	MET
1	F	1	MET
1	F	132	PRO
1	F	136	LYS
1	F	139	ASP
1	F	170	LYS
1	F	214	ASP
1	F	215	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	143	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	HEM	C	302	1,5	41,50,50	1.47	5 (12%)	45,82,82	1.30	5 (11%)
3	HEM	B	302	1,5	41,50,50	1.52	8 (19%)	45,82,82	1.34	3 (6%)
3	HEM	A	302	1,5	41,50,50	1.50	4 (9%)	45,82,82	1.48	8 (17%)
3	HEM	F	302	1,5	41,50,50	1.50	5 (12%)	45,82,82	1.52	7 (15%)
3	HEM	E	302	1,5	41,50,50	1.46	5 (12%)	45,82,82	1.44	7 (15%)
2	ASC	E	301	-	12,12,12	3.13	4 (33%)	17,17,17	2.09	5 (29%)
2	ASC	C	301	-	12,12,12	3.20	6 (50%)	17,17,17	2.23	6 (35%)
3	HEM	D	302	1,5	41,50,50	1.51	6 (14%)	45,82,82	1.55	9 (20%)
2	ASC	F	301	-	12,12,12	2.84	4 (33%)	17,17,17	2.77	9 (52%)
2	ASC	D	301	-	12,12,12	3.04	5 (41%)	17,17,17	2.36	6 (35%)
2	ASC	A	301	-	12,12,12	2.95	5 (41%)	17,17,17	2.39	4 (23%)
2	ASC	B	301	-	12,12,12	3.00	5 (41%)	17,17,17	2.40	8 (47%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	C	302	1,5	-	6/12/54/54	-
3	HEM	B	302	1,5	-	2/12/54/54	-
3	HEM	A	302	1,5	-	5/12/54/54	-
3	HEM	F	302	1,5	-	2/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	E	302	1,5	-	2/12/54/54	-
2	ASC	E	301	-	-	2/6/22/22	0/1/1/1
2	ASC	C	301	-	-	2/6/22/22	0/1/1/1
3	HEM	D	302	1,5	-	2/12/54/54	-
2	ASC	F	301	-	-	6/6/22/22	0/1/1/1
2	ASC	D	301	-	-	0/6/22/22	0/1/1/1
2	ASC	A	301	-	-	0/6/22/22	0/1/1/1
2	ASC	B	301	-	-	3/6/22/22	0/1/1/1

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	ASC	O4-C1	9.15	1.49	1.36
2	E	301	ASC	O4-C1	8.98	1.49	1.36
2	D	301	ASC	O4-C1	8.82	1.49	1.36
2	B	301	ASC	O4-C1	8.61	1.49	1.36
2	A	301	ASC	O4-C1	8.39	1.48	1.36
2	F	301	ASC	O4-C1	8.09	1.48	1.36
3	A	302	HEM	C3C-C2C	-4.37	1.34	1.40
3	C	302	HEM	C3C-C2C	-4.28	1.34	1.40
3	E	302	HEM	C3C-C2C	-4.17	1.34	1.40
3	D	302	HEM	C3C-C2C	-4.16	1.34	1.40
3	F	302	HEM	C3C-C2C	-4.13	1.34	1.40
3	B	302	HEM	C3C-C2C	-4.03	1.34	1.40
3	F	302	HEM	C3C-CAC	3.75	1.55	1.47
3	B	302	HEM	FE-ND	3.46	2.14	1.96
3	A	302	HEM	C3C-CAC	3.46	1.54	1.47
3	D	302	HEM	C3C-CAC	3.46	1.54	1.47
2	C	301	ASC	O4-C4	3.46	1.51	1.45
2	E	301	ASC	O4-C4	3.40	1.51	1.45
3	B	302	HEM	C3C-CAC	3.29	1.54	1.47
3	C	302	HEM	C3C-CAC	3.26	1.54	1.47
3	E	302	HEM	C3C-CAC	3.16	1.54	1.47
2	D	301	ASC	O4-C4	3.13	1.51	1.45
3	A	302	HEM	CAB-C3B	2.94	1.55	1.47
2	F	301	ASC	O3-C3	2.94	1.42	1.33
3	C	302	HEM	CAB-C3B	2.84	1.55	1.47
2	F	301	ASC	O4-C4	2.83	1.50	1.45
3	E	302	HEM	CAB-C3B	2.82	1.55	1.47
3	D	302	HEM	CAB-C3B	2.79	1.55	1.47
3	B	302	HEM	CAB-C3B	2.76	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	ASC	O3-C3	2.76	1.41	1.33
2	B	301	ASC	O4-C4	2.74	1.50	1.45
2	B	301	ASC	O3-C3	2.73	1.41	1.33
2	C	301	ASC	C5-C4	-2.71	1.48	1.53
2	E	301	ASC	O3-C3	2.66	1.41	1.33
3	F	302	HEM	CAB-C3B	2.65	1.54	1.47
2	D	301	ASC	O3-C3	2.63	1.41	1.33
2	A	301	ASC	O4-C4	2.61	1.50	1.45
2	C	301	ASC	O3-C3	2.59	1.41	1.33
3	C	302	HEM	FE-ND	2.55	2.09	1.96
2	A	301	ASC	C5-C4	-2.46	1.48	1.53
3	E	302	HEM	FE-ND	2.46	2.09	1.96
2	B	301	ASC	O2-C2	2.43	1.41	1.33
3	D	302	HEM	FE-ND	2.39	2.08	1.96
2	B	301	ASC	C5-C4	-2.33	1.48	1.53
2	E	301	ASC	C5-C4	-2.31	1.48	1.53
2	C	301	ASC	O2-C2	2.27	1.41	1.33
3	D	302	HEM	FE-NB	2.19	2.07	1.96
2	F	301	ASC	O2-C2	2.18	1.41	1.33
2	A	301	ASC	C4-C3	-2.18	1.46	1.50
2	D	301	ASC	C5-C4	-2.15	1.49	1.53
3	B	302	HEM	CMD-C2D	2.15	1.55	1.50
2	C	301	ASC	C4-C3	-2.14	1.46	1.50
2	D	301	ASC	O2-C2	2.13	1.40	1.33
3	D	302	HEM	CMD-C2D	2.10	1.55	1.50
3	F	302	HEM	FE-ND	2.10	2.07	1.96
3	B	302	HEM	CAA-C2A	2.08	1.55	1.52
3	A	302	HEM	CMB-C2B	2.07	1.55	1.50
3	C	302	HEM	CMB-C2B	2.03	1.55	1.50
3	F	302	HEM	CMD-C2D	2.02	1.55	1.50
3	E	302	HEM	CAA-C2A	2.01	1.55	1.52
3	B	302	HEM	CAD-C3D	2.01	1.56	1.51
3	B	302	HEM	CMB-C2B	2.00	1.55	1.50

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	ASC	O4-C1-C2	-5.69	104.80	109.86
2	D	301	ASC	O4-C1-O1	5.62	127.89	121.25
2	F	301	ASC	O4-C1-C2	-5.31	105.14	109.86
2	C	301	ASC	O4-C1-C2	-5.20	105.24	109.86
2	D	301	ASC	O4-C1-C2	-5.01	105.41	109.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	ASC	O4-C1-O1	4.78	126.89	121.25
2	F	301	ASC	O4-C1-O1	4.74	126.85	121.25
2	F	301	ASC	O3-C3-C2	-4.72	119.89	132.29
2	B	301	ASC	O4-C1-C2	-4.54	105.82	109.86
2	E	301	ASC	O4-C1-C2	-4.50	105.86	109.86
2	C	301	ASC	O4-C1-O1	4.44	126.49	121.25
2	B	301	ASC	O3-C3-C2	-4.18	121.31	132.29
2	E	301	ASC	O4-C1-O1	4.04	126.02	121.25
2	B	301	ASC	O4-C1-O1	3.80	125.74	121.25
2	A	301	ASC	O3-C3-C2	-3.76	122.42	132.29
2	A	301	ASC	C5-C4-C3	-3.69	107.77	114.78
3	E	302	HEM	CHC-C4B-NB	3.62	128.36	124.43
3	A	302	HEM	C4C-CHD-C1D	3.61	127.32	122.56
2	F	301	ASC	C1-C2-C3	3.54	112.30	107.80
3	E	302	HEM	C4B-CHC-C1C	3.42	127.07	122.56
2	B	301	ASC	O5-C5-C4	3.40	117.48	110.77
3	F	302	HEM	CBA-CAA-C2A	-3.23	107.10	112.62
2	E	301	ASC	O3-C3-C2	-3.20	123.87	132.29
2	D	301	ASC	C5-C4-C3	-3.15	108.80	114.78
3	D	302	HEM	C1B-NB-C4B	3.15	108.33	105.07
2	D	301	ASC	O3-C3-C2	-3.06	124.23	132.29
2	B	301	ASC	C6-C5-C4	-3.05	106.61	111.86
2	E	301	ASC	C6-C5-C4	-2.99	106.72	111.86
2	F	301	ASC	C5-C4-C3	-2.92	109.25	114.78
3	B	302	HEM	CMC-C2C-C3C	2.91	130.11	124.68
3	E	302	HEM	C4D-ND-C1D	2.90	108.07	105.07
3	F	302	HEM	C4C-CHD-C1D	2.89	126.37	122.56
3	A	302	HEM	CMC-C2C-C3C	2.88	130.06	124.68
3	A	302	HEM	CAD-CBD-CGD	-2.85	107.48	113.60
3	F	302	HEM	C1B-NB-C4B	2.83	108.00	105.07
3	D	302	HEM	C4B-CHC-C1C	2.83	126.29	122.56
3	D	302	HEM	C4C-CHD-C1D	2.81	126.26	122.56
2	B	301	ASC	C4-O4-C1	-2.80	106.09	109.25
2	F	301	ASC	C6-C5-C4	-2.78	107.07	111.86
2	F	301	ASC	O5-C5-C4	2.75	116.19	110.77
3	D	302	HEM	C4D-ND-C1D	2.71	107.87	105.07
3	C	302	HEM	CAA-CBA-CGA	-2.70	106.19	113.76
3	F	302	HEM	C4B-CHC-C1C	2.70	126.12	122.56
3	B	302	HEM	CMA-C3A-C4A	-2.60	124.47	128.46
2	C	301	ASC	O3-C3-C2	-2.57	125.54	132.29
3	F	302	HEM	C4D-ND-C1D	2.51	107.67	105.07
3	F	302	HEM	C3B-C2B-C1B	2.50	108.34	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	302	HEM	CBA-CAA-C2A	-2.50	108.36	112.62
2	C	301	ASC	C1-C2-C3	2.49	110.96	107.80
3	C	302	HEM	C4C-CHD-C1D	2.49	125.85	122.56
2	E	301	ASC	O2-C2-C3	-2.45	121.13	128.44
2	C	301	ASC	C5-C4-C3	-2.45	110.13	114.78
3	A	302	HEM	CHC-C4B-NB	2.41	127.05	124.43
3	A	302	HEM	CAA-CBA-CGA	-2.40	107.02	113.76
2	C	301	ASC	C6-C5-C4	-2.40	107.72	111.86
3	A	302	HEM	CAD-C3D-C4D	2.40	128.85	124.66
2	B	301	ASC	O2-C2-C3	-2.36	121.41	128.44
3	B	302	HEM	C4C-CHD-C1D	2.33	125.63	122.56
3	D	302	HEM	CMC-C2C-C3C	2.29	128.97	124.68
2	F	301	ASC	O3-C3-C4	2.28	124.04	118.08
2	D	301	ASC	O3-C3-C4	2.22	123.87	118.08
3	E	302	HEM	C1D-C2D-C3D	2.19	109.26	106.96
2	B	301	ASC	C5-C4-C3	-2.18	110.64	114.78
3	C	302	HEM	CMC-C2C-C3C	2.15	128.71	124.68
3	E	302	HEM	C4C-CHD-C1D	2.15	125.40	122.56
3	A	302	HEM	O1D-CGD-CBD	-2.13	116.23	123.08
3	D	302	HEM	O2D-CGD-CBD	2.09	120.75	114.03
2	D	301	ASC	O2-C2-C3	-2.08	122.23	128.44
2	F	301	ASC	C4-O4-C1	-2.07	106.91	109.25
3	D	302	HEM	C3B-C2B-C1B	2.07	108.02	106.49
3	C	302	HEM	C1B-NB-C4B	2.07	107.21	105.07
3	D	302	HEM	CMA-C3A-C4A	-2.06	125.29	128.46
3	E	302	HEM	C1B-NB-C4B	2.06	107.20	105.07
3	E	302	HEM	CMC-C2C-C3C	2.05	128.51	124.68
3	A	302	HEM	CHD-C1D-ND	2.04	126.65	124.43
3	C	302	HEM	C2C-C3C-C4C	2.03	108.32	106.90
3	F	302	HEM	CHC-C4B-C3B	2.02	127.66	124.57

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	ASC	C4-C5-C6-O6
2	F	301	ASC	C3-C4-C5-O5
2	F	301	ASC	O4-C4-C5-C6
2	F	301	ASC	O4-C4-C5-O5
2	F	301	ASC	C4-C5-C6-O6
2	F	301	ASC	O5-C5-C6-O6
2	B	301	ASC	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	E	301	ASC	C4-C5-C6-O6
2	C	301	ASC	C4-C5-C6-O6
2	E	301	ASC	O5-C5-C6-O6
2	C	301	ASC	O5-C5-C6-O6
3	A	302	HEM	C1A-C2A-CAA-CBA
3	A	302	HEM	C3A-C2A-CAA-CBA
3	C	302	HEM	C1A-C2A-CAA-CBA
3	C	302	HEM	C3A-C2A-CAA-CBA
3	A	302	HEM	CAA-CBA-CGA-O1A
3	C	302	HEM	CAA-CBA-CGA-O1A
2	F	301	ASC	C3-C4-C5-C6
3	D	302	HEM	CAA-CBA-CGA-O1A
3	F	302	HEM	CAA-CBA-CGA-O1A
3	E	302	HEM	CAA-CBA-CGA-O1A
3	C	302	HEM	CAA-CBA-CGA-O2A
3	E	302	HEM	CAA-CBA-CGA-O2A
3	D	302	HEM	CAA-CBA-CGA-O2A
3	C	302	HEM	CAD-CBD-CGD-O2D
3	F	302	HEM	CAA-CBA-CGA-O2A
3	A	302	HEM	CAA-CBA-CGA-O2A
3	C	302	HEM	CAD-CBD-CGD-O1D
2	B	301	ASC	O4-C4-C5-O5
3	A	302	HEM	CAD-CBD-CGD-O2D
3	B	302	HEM	CAD-CBD-CGD-O2D
3	B	302	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

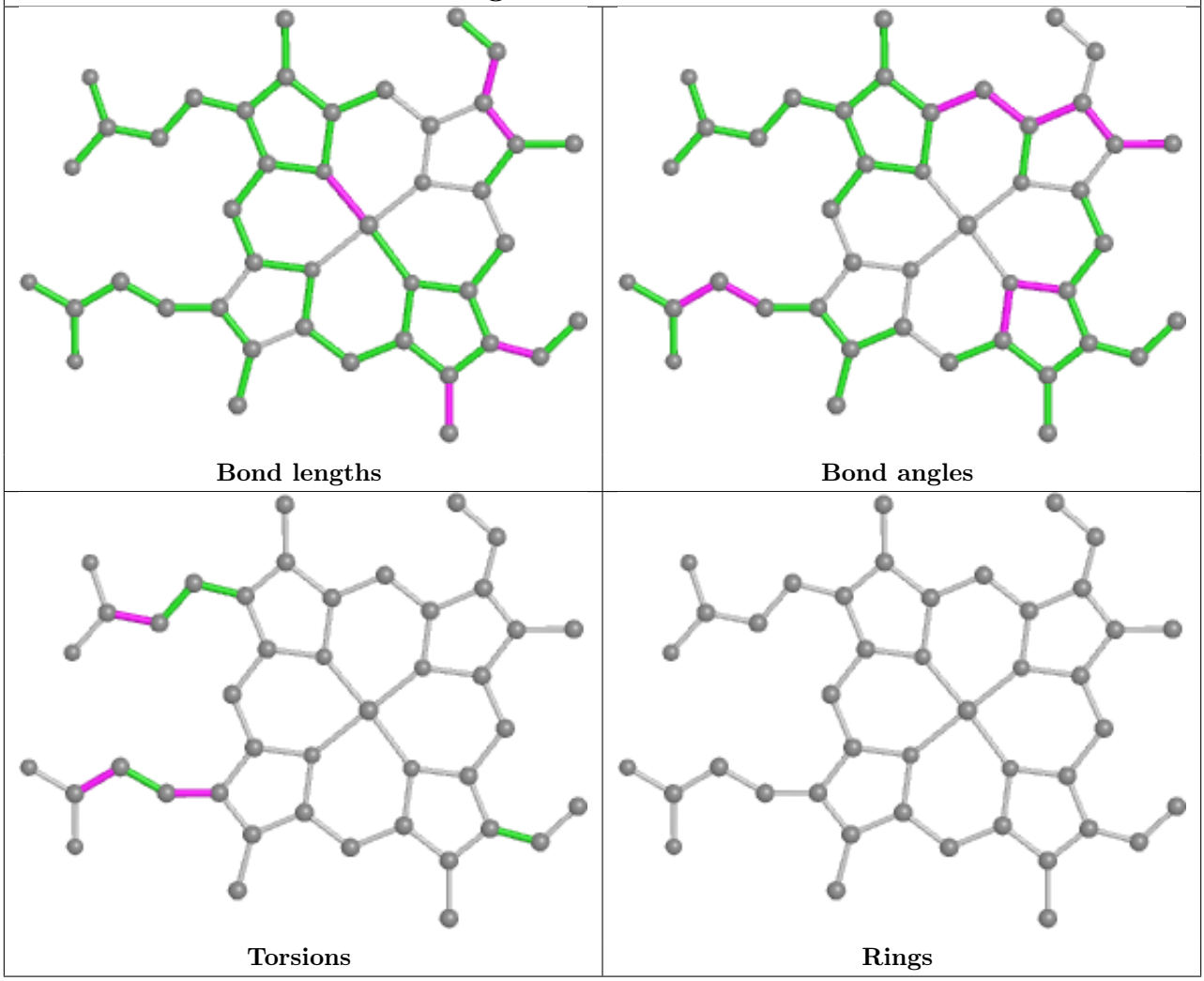
8 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	302	HEM	4	0
3	B	302	HEM	6	0
3	A	302	HEM	6	0
3	F	302	HEM	7	0
3	E	302	HEM	5	0
3	D	302	HEM	3	0
2	D	301	ASC	1	0
2	A	301	ASC	1	0

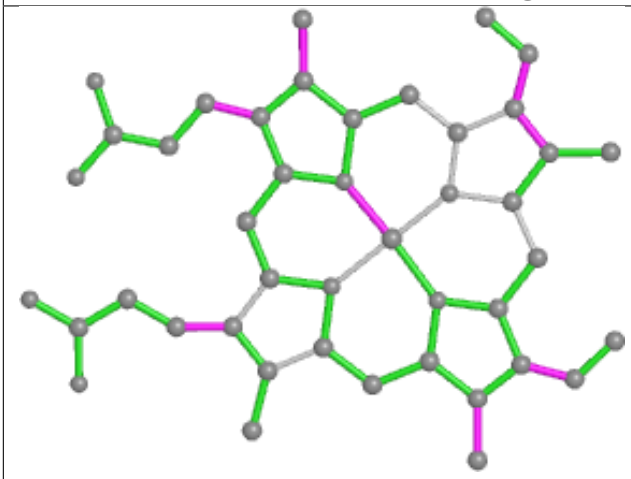
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

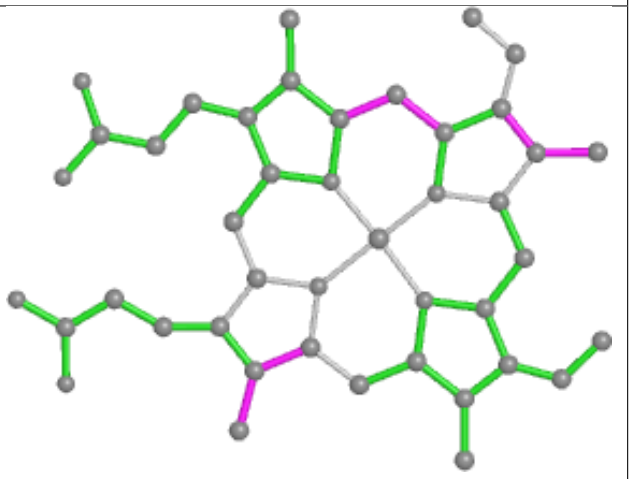
Ligand HEM C 302



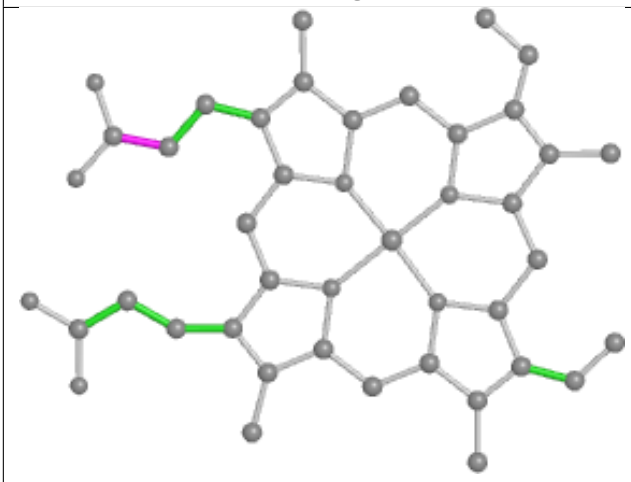
Ligand HEM B 302



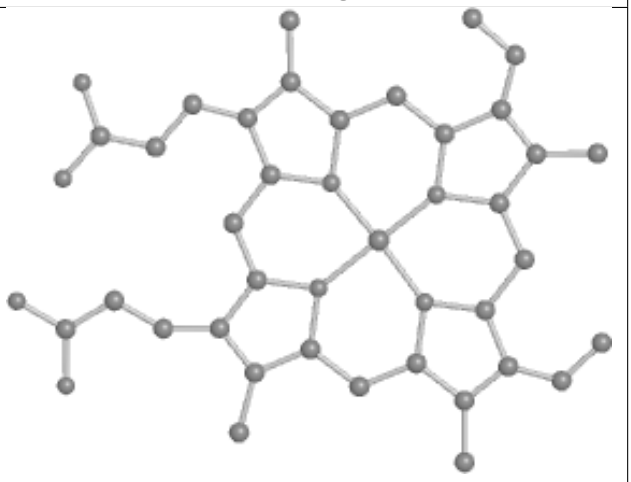
Bond lengths



Bond angles

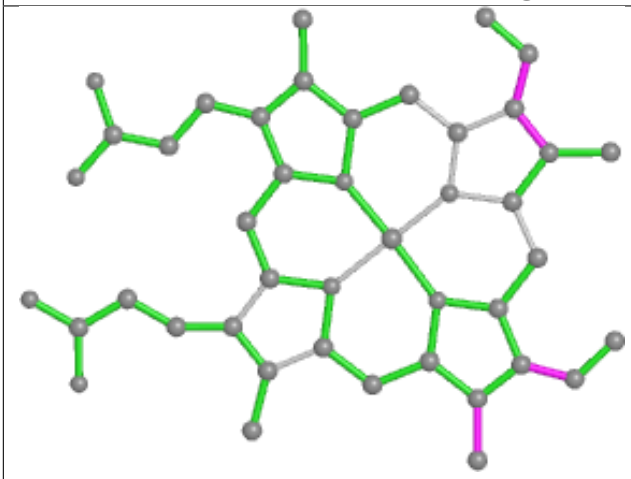


Torsions

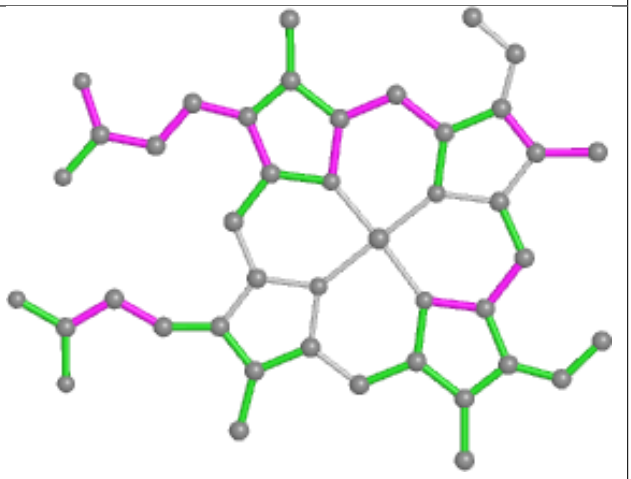


Rings

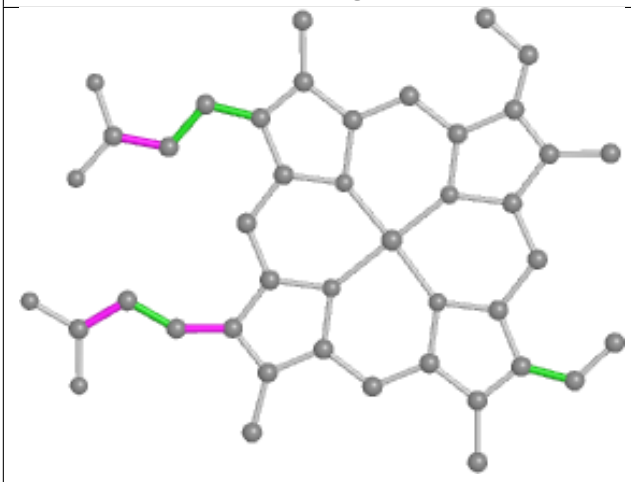
Ligand HEM A 302



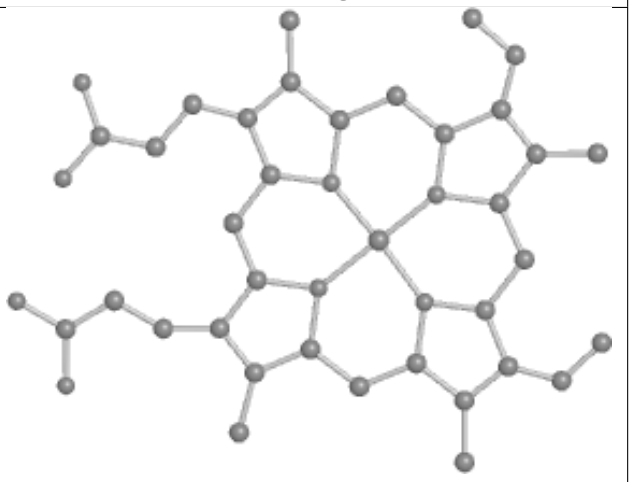
Bond lengths



Bond angles

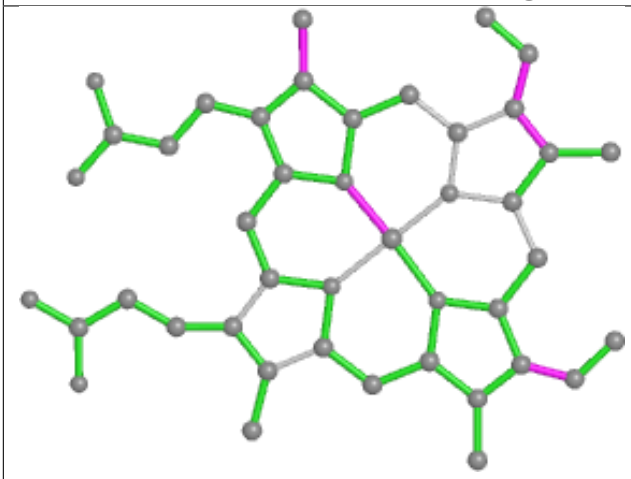


Torsions

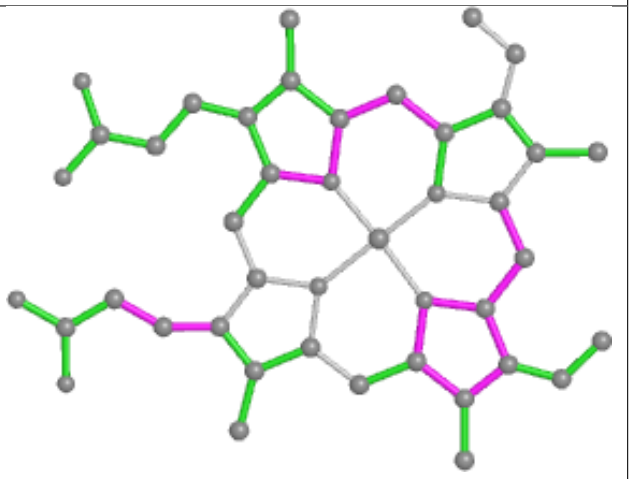


Rings

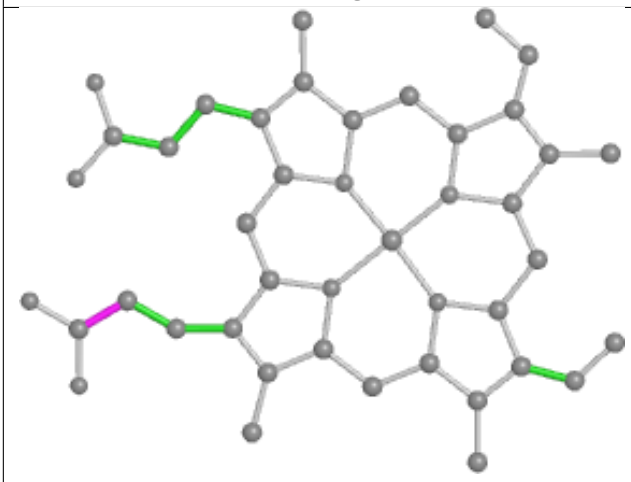
Ligand HEM F 302



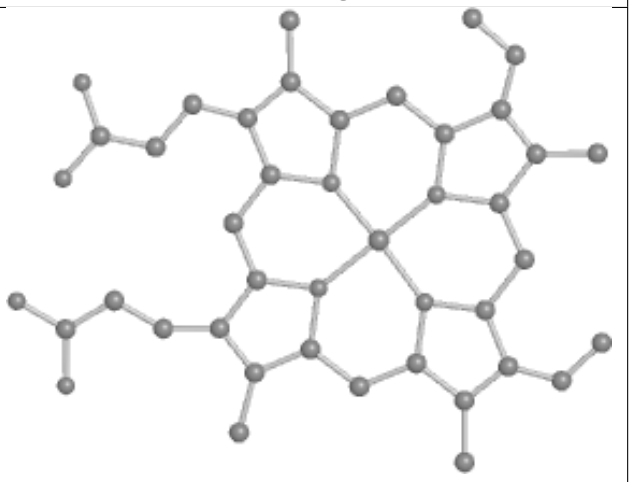
Bond lengths



Bond angles

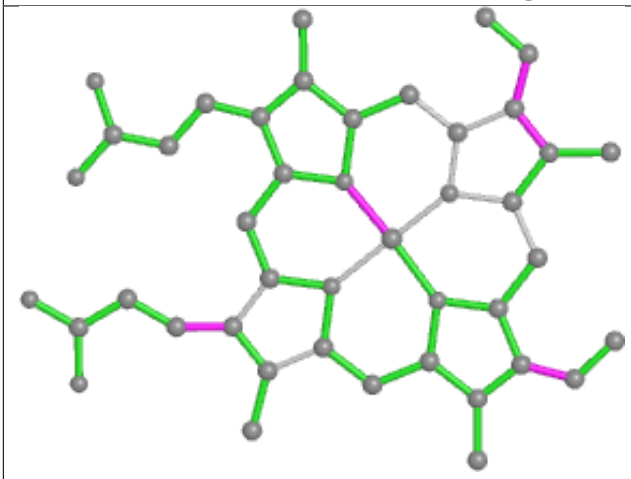


Torsions

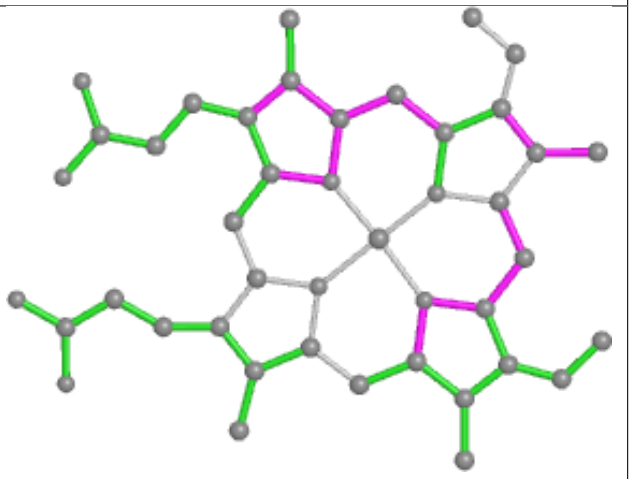


Rings

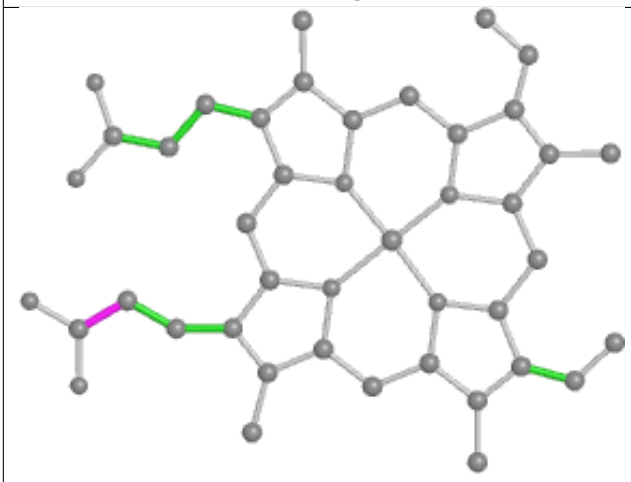
Ligand HEM E 302



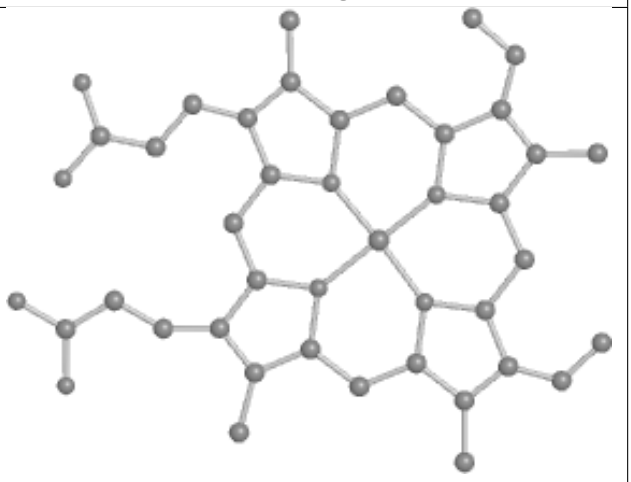
Bond lengths



Bond angles

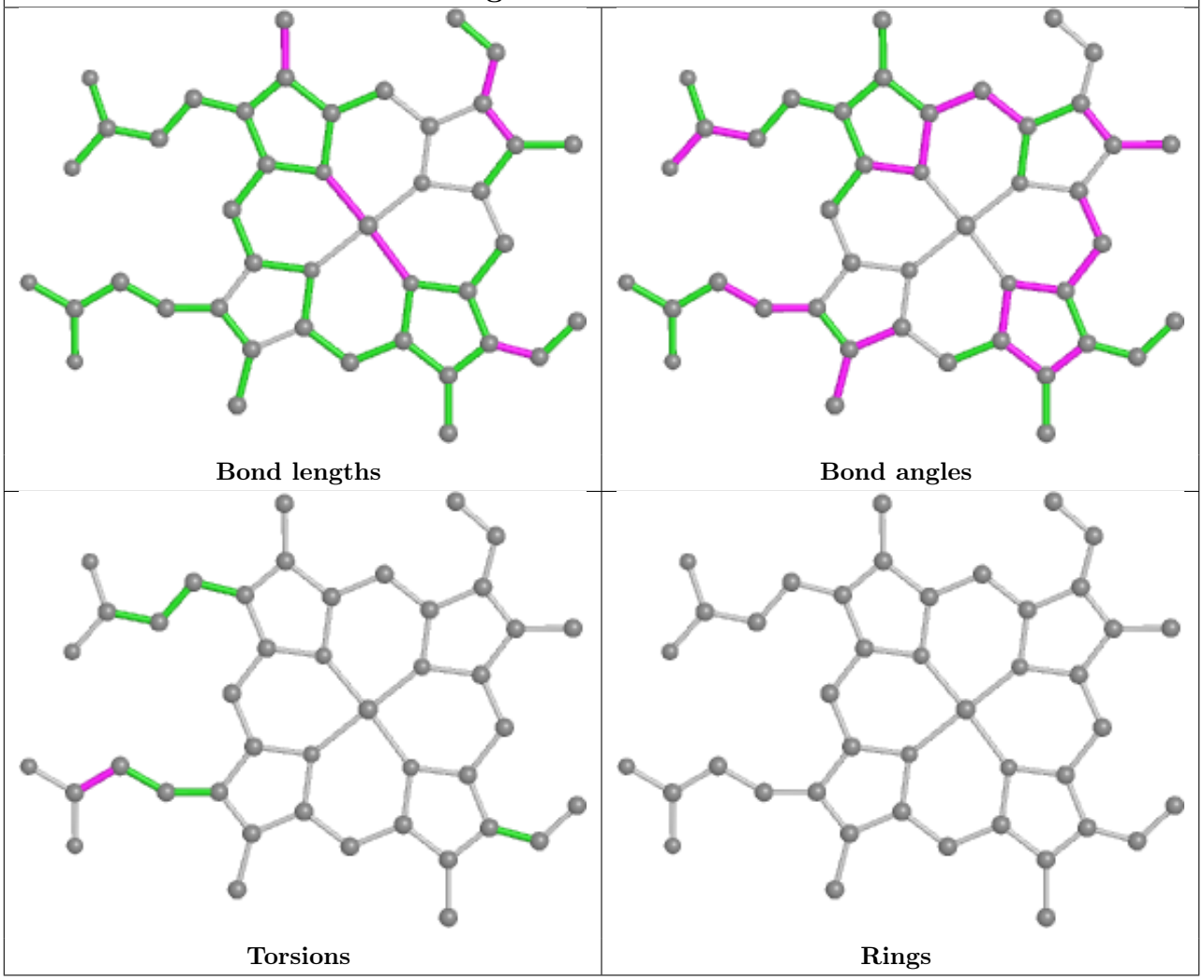


Torsions



Rings

Ligand HEM D 302



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, 95^{th} 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	250/250 (100%)	-0.46	1 (0%) 92 91	18, 27, 38, 58	0
1	B	250/250 (100%)	-0.36	0 100 100	19, 32, 47, 65	0
1	C	250/250 (100%)	-0.34	0 100 100	21, 33, 46, 57	0
1	D	250/250 (100%)	-0.52	0 100 100	19, 28, 41, 63	0
1	E	250/250 (100%)	-0.37	0 100 100	22, 33, 47, 57	0
1	F	250/250 (100%)	-0.25	2 (0%) 86 85	22, 36, 57, 76	0
All	All	1500/1500 (100%)	-0.38	3 (0%) 95 94	18, 31, 49, 76	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	124	GLN	2.7
1	F	135	THR	2.4
1	F	124	GLN	2.1

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

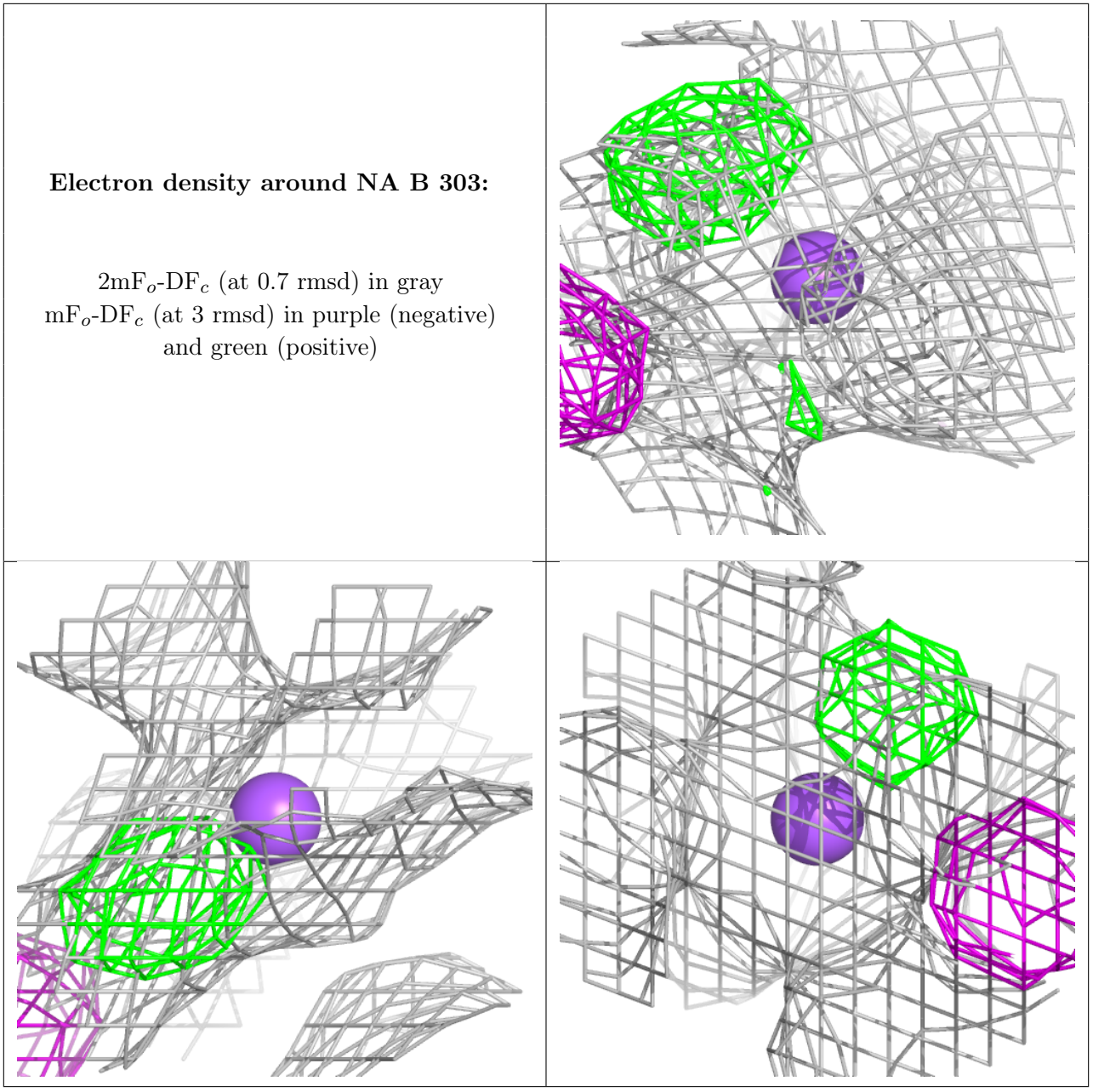
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ASC	B	301	12/12	0.90	0.13	30,37,46,48	0
2	ASC	F	301	12/12	0.91	0.09	35,44,55,55	0
2	ASC	E	301	12/12	0.92	0.14	31,39,49,53	0
2	ASC	C	301	12/12	0.93	0.17	36,45,56,58	0
2	ASC	A	301	12/12	0.94	0.10	24,35,46,54	0
4	NA	B	303	1/1	0.94	0.13	26,26,26,26	0
2	ASC	D	301	12/12	0.95	0.14	29,37,47,56	0
4	NA	F	303	1/1	0.96	0.10	36,36,36,36	0
3	HEM	D	302	43/43	0.97	0.12	22,30,40,41	0
3	HEM	E	302	43/43	0.97	0.09	24,31,39,50	0
3	HEM	F	302	43/43	0.97	0.11	30,39,51,53	0
4	NA	A	303	1/1	0.97	0.12	24,24,24,24	0
3	HEM	B	302	43/43	0.97	0.11	25,36,53,59	0
4	NA	E	303	1/1	0.97	0.06	30,30,30,30	0
3	HEM	C	302	43/43	0.97	0.11	26,36,51,54	0
3	HEM	A	302	43/43	0.98	0.10	19,26,37,40	0
4	NA	C	303	1/1	0.98	0.07	32,32,32,32	0
4	NA	D	303	1/1	0.99	0.07	25,25,25,25	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.

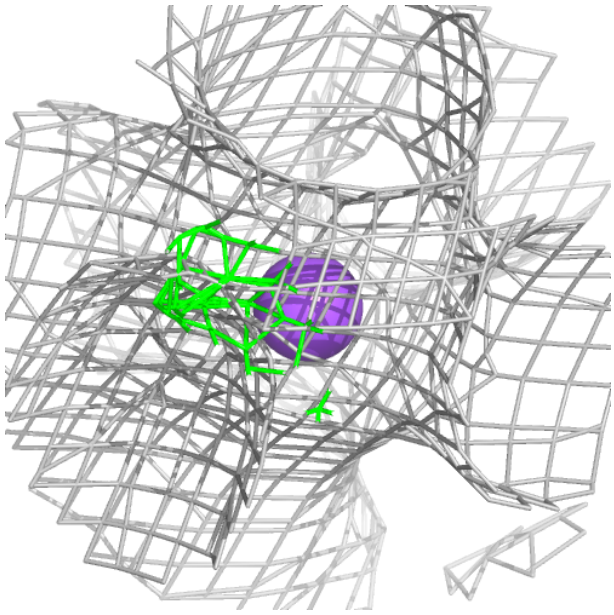
Electron density around NA B 303:

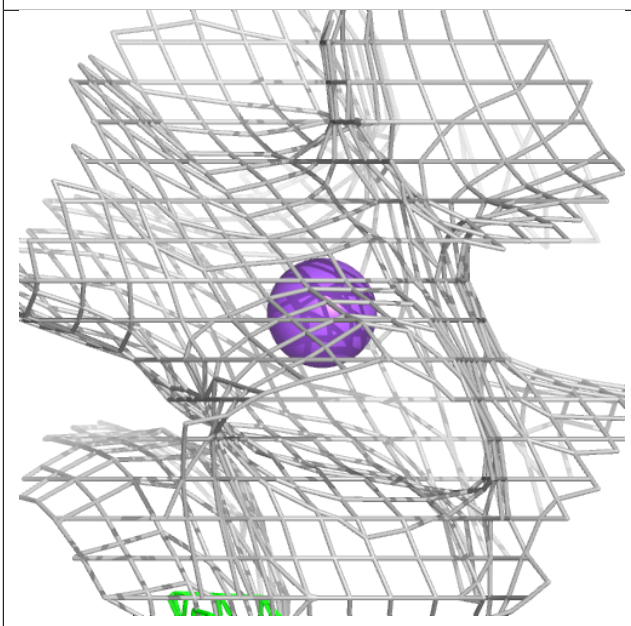
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

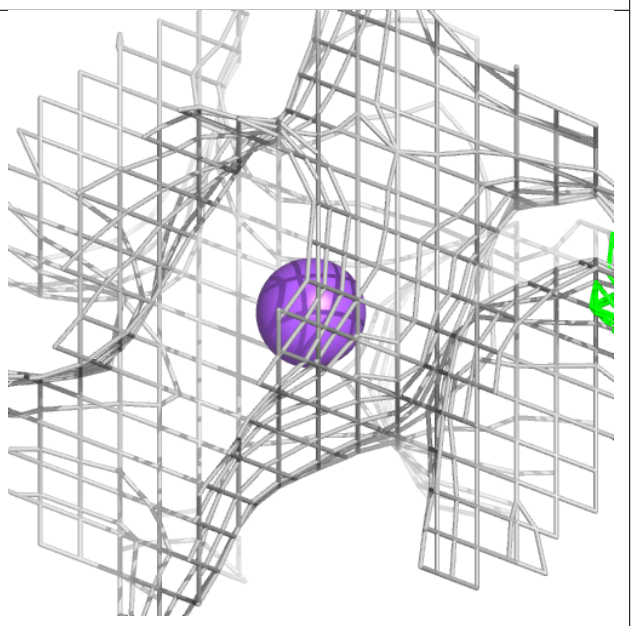


Electron density around NA F 303:

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

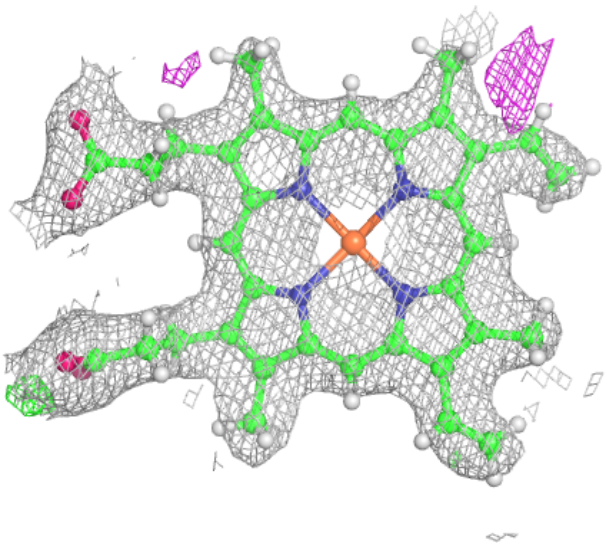


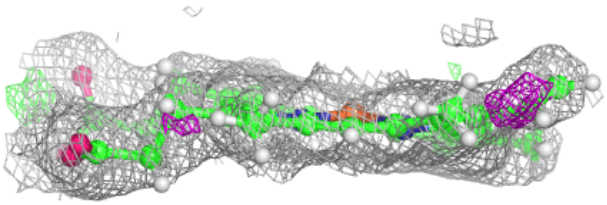


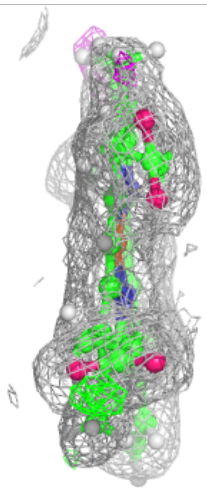


Electron density around HEM D 302:

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

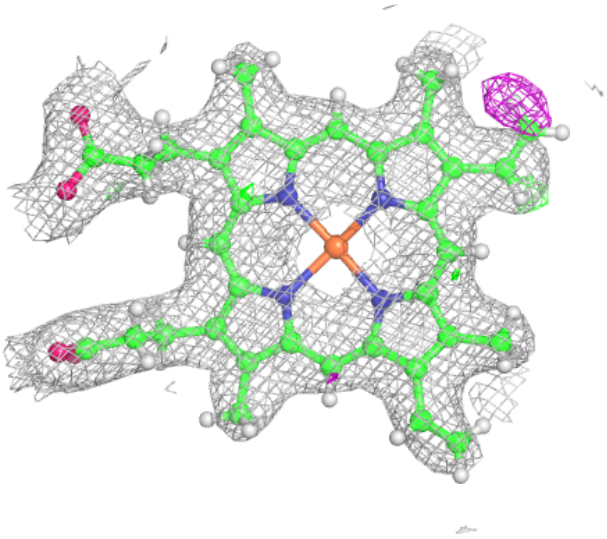


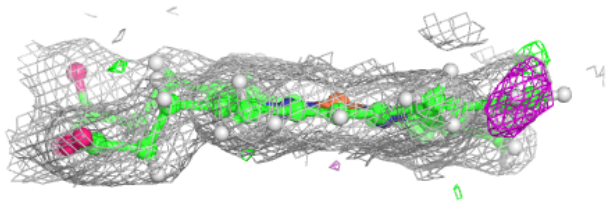


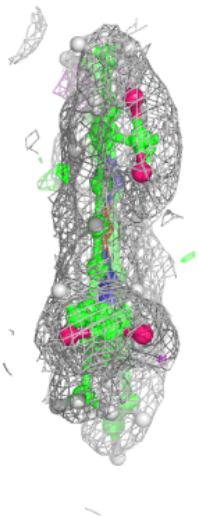


Electron density around HEM E 302:

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

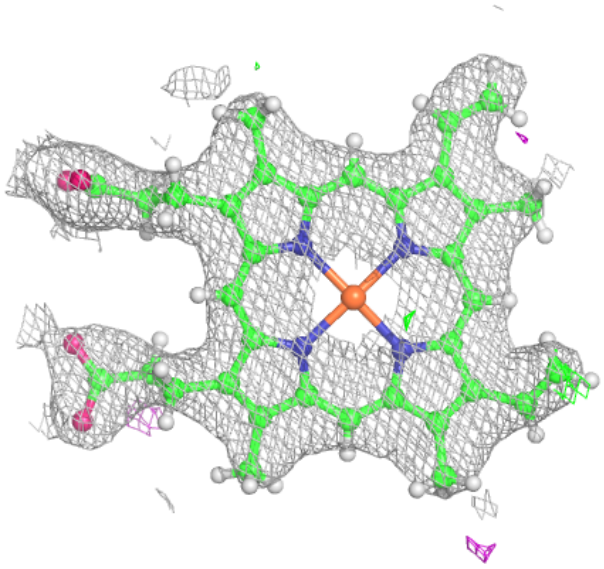


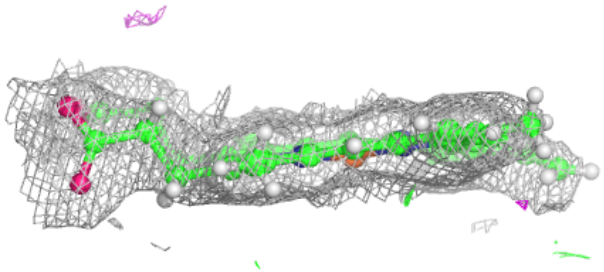


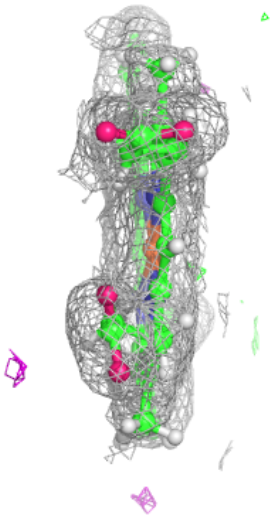


Electron density around HEM F 302:

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

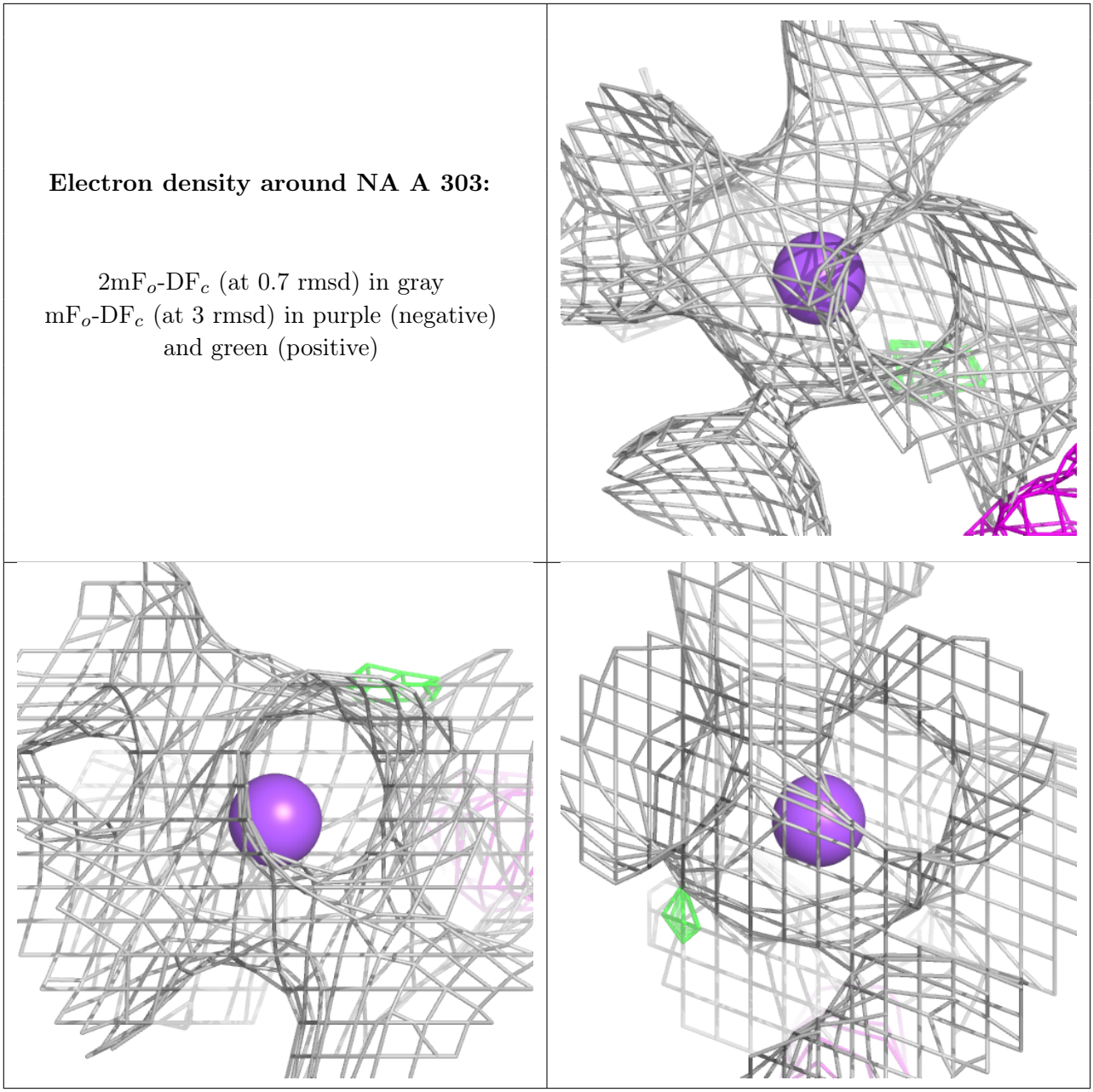






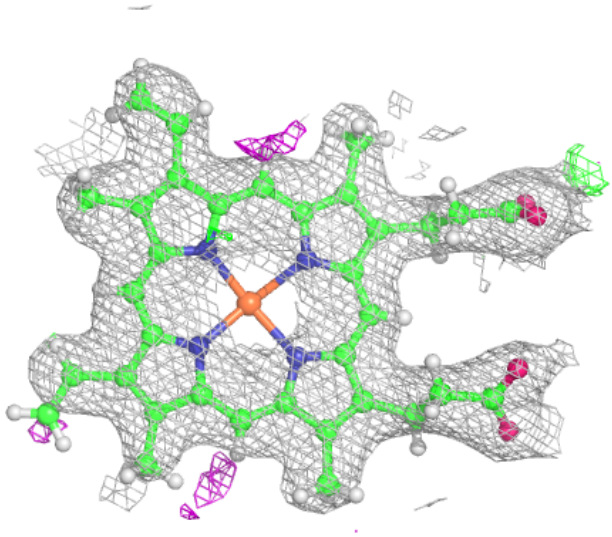
Electron density around NA A 303:

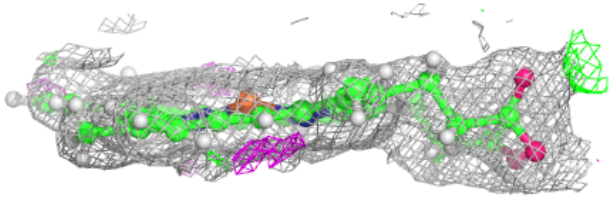
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

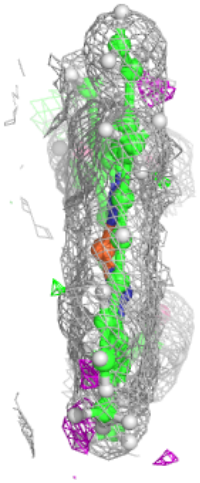


Electron density around HEM B 302:

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

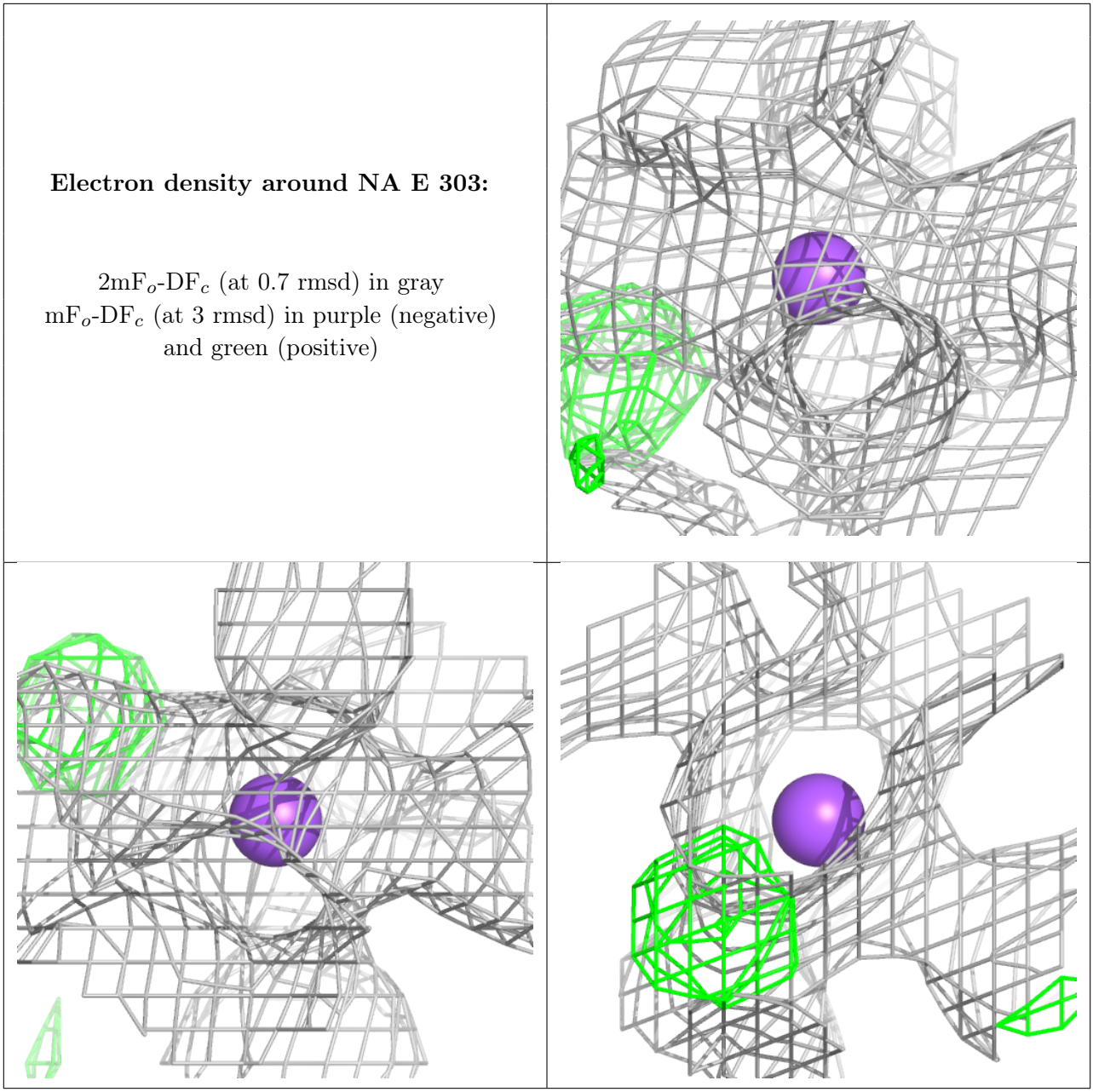






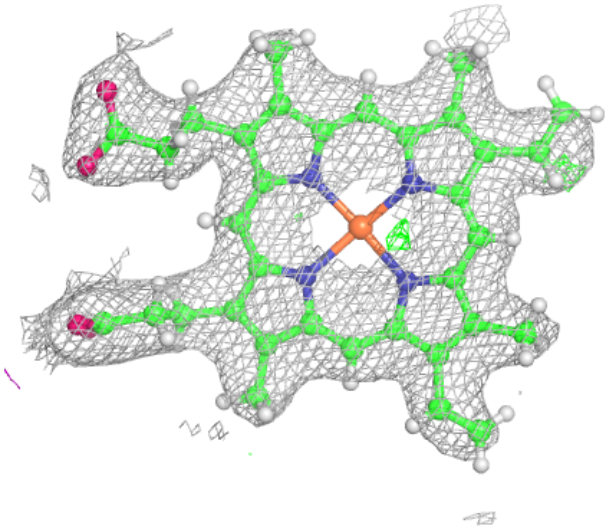
Electron density around NA E 303:

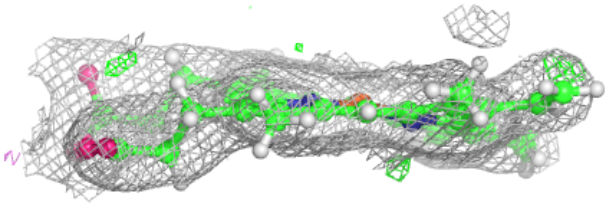
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

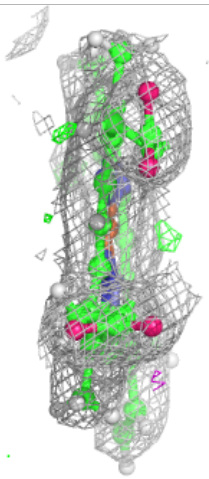


Electron density around HEM C 302:

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

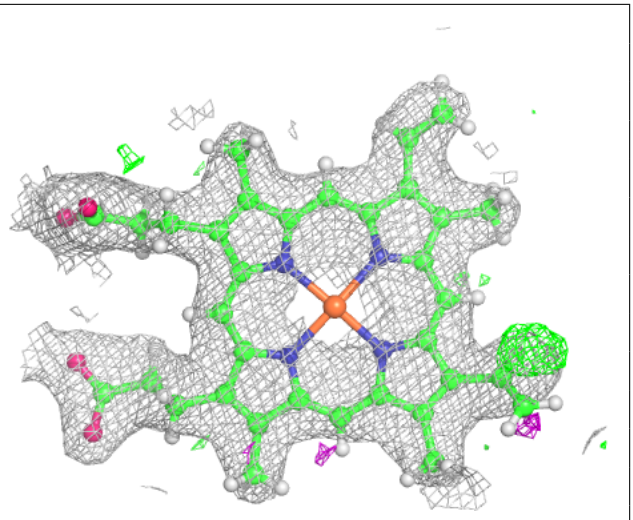


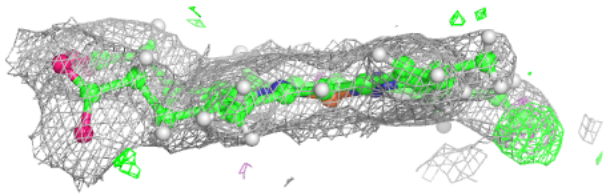


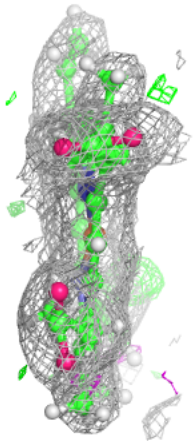


Electron density around HEM A 302:

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

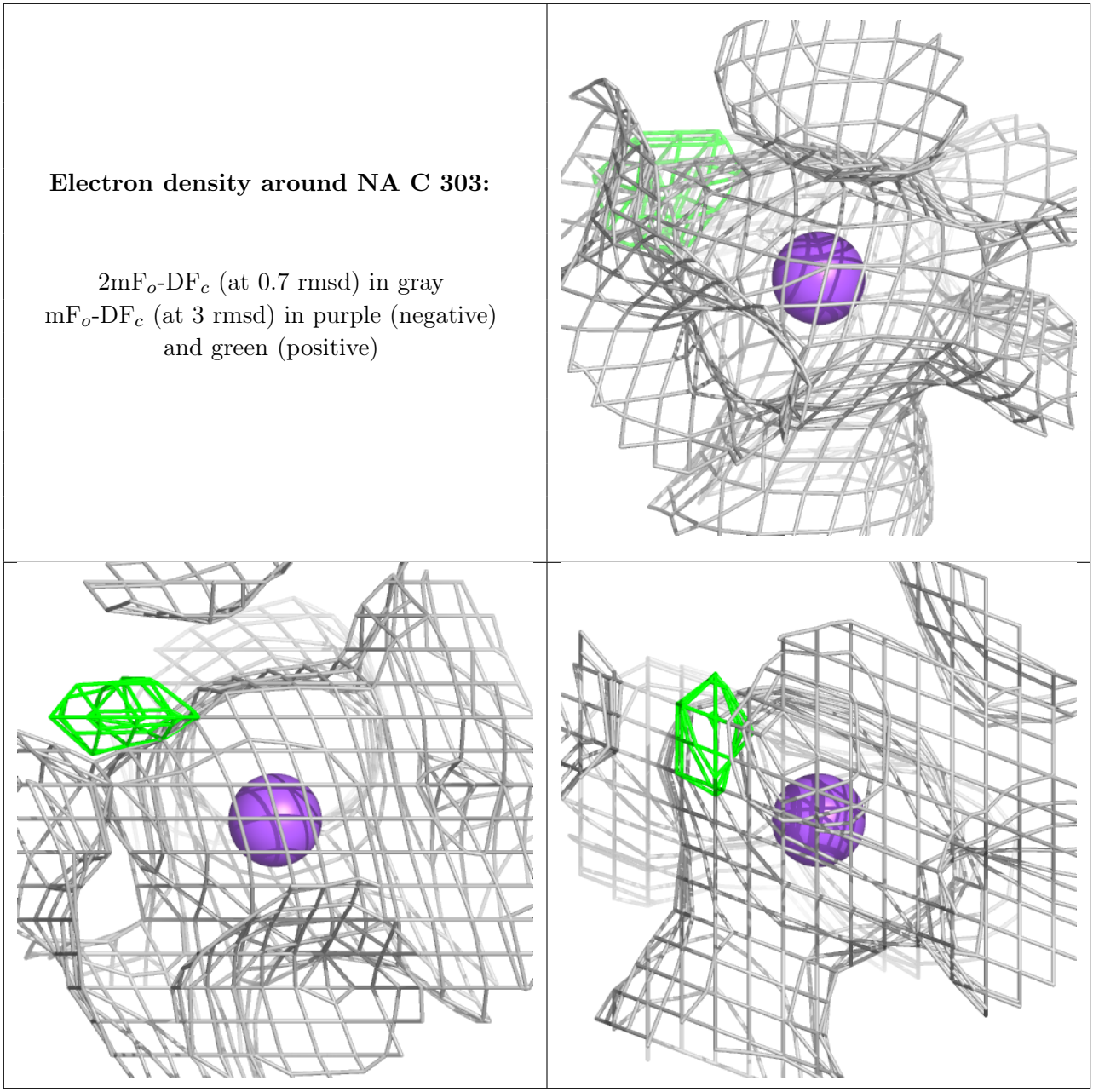






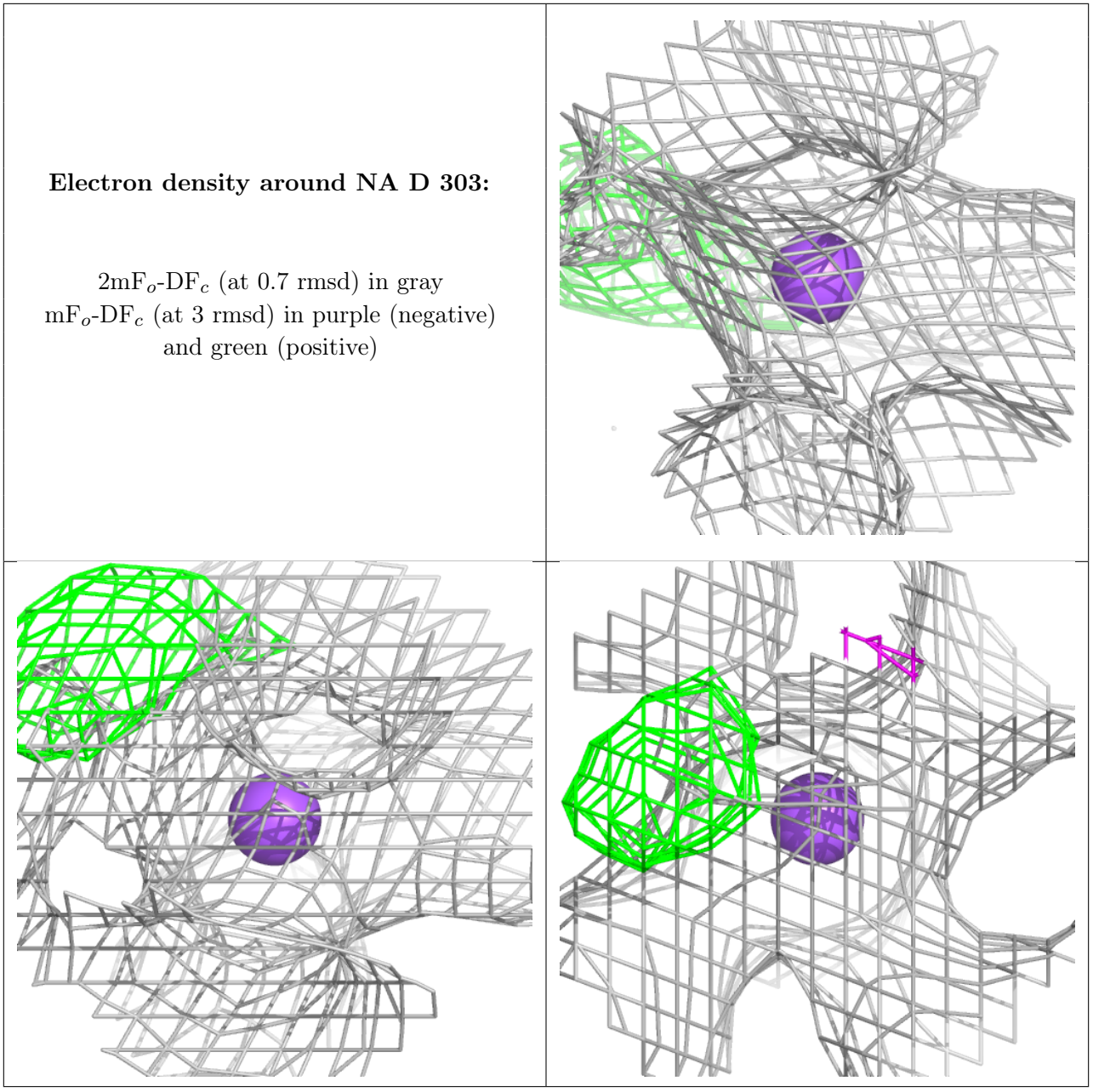
Electron density around NA C 303:

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



Electron density around NA D 303:

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



6.5 Other polymers

There are no such residues in this entry.