



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:04 PM UTC

PDB ID : 8FF7 / pdb\_00008ff7  
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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (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

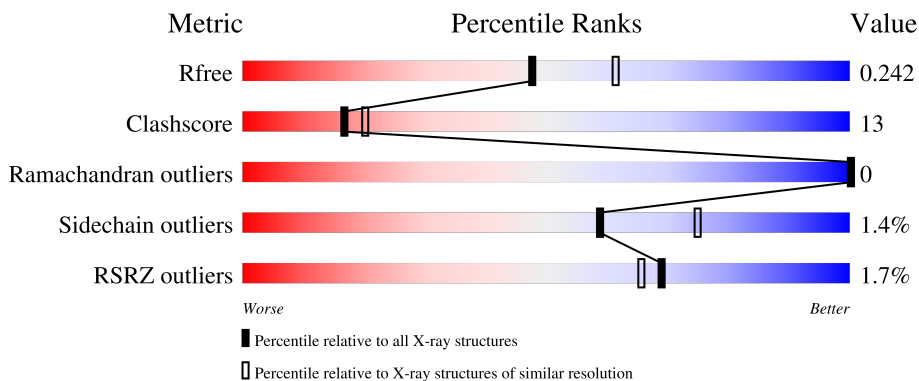
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 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.



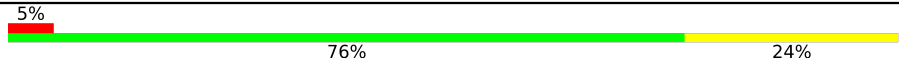
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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  $\geq 3$ , 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	250	 81% 18%
1	B	250	 76% 23%
1	C	250	 79% 21%
1	D	250	 83% 17%
1	E	250	 74% 26%

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Mol	Chain	Length	Quality of chain
1	F	250	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a small red segment on the left labeled '5%', a large green segment in the middle labeled '76%', and a yellow segment on the right labeled '24%'.</p>

## 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
			Total	C	N	O	S			
1	A	250	1923	1219	331	367	6	0	0	0
1	B	250	1923	1219	331	367	6	0	0	0
1	C	250	1923	1219	331	367	6	0	0	0
1	D	250	1923	1219	331	367	6	0	0	0
1	E	250	1923	1219	331	367	6	0	0	0
1	F	250	1923	1219	331	367	6	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

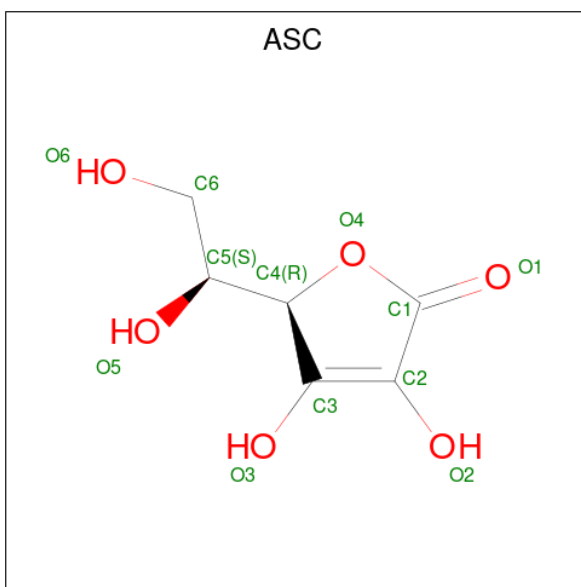
Chain	Residue	Modelled	Actual	Comment	Reference
A	4	SER	CYS	engineered mutation	UNP A0A8T0NWI5
A	14	ASP	GLU	engineered mutation	UNP A0A8T0NWI5
A	168	ALA	CYS	engineered mutation	UNP A0A8T0NWI5
A	221	ALA	VAL	engineered mutation	UNP A0A8T0NWI5
A	229	ASP	LYS	engineered mutation	UNP A0A8T0NWI5
B	4	SER	CYS	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 (CCD ID: ASC) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>6</sub>).



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

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

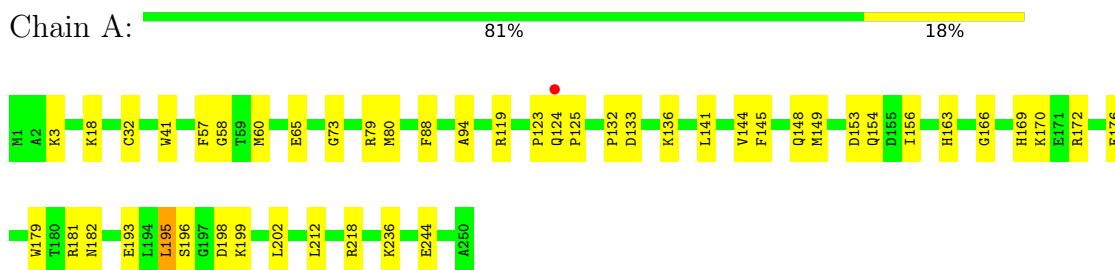
- Molecule 5 is water.

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

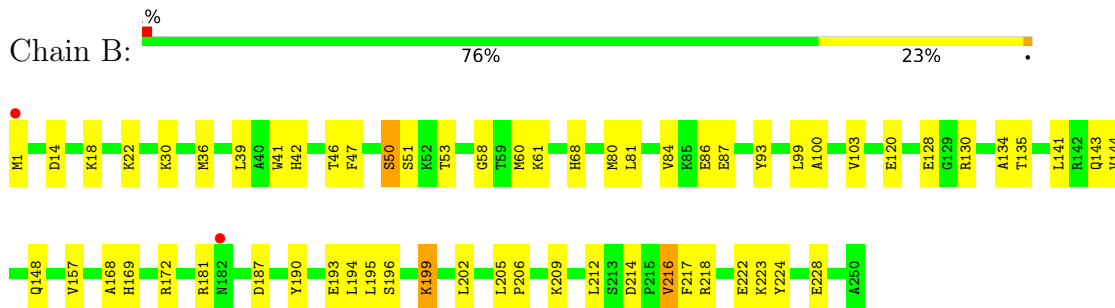
### 3 Residue-property plots [i](#)

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.

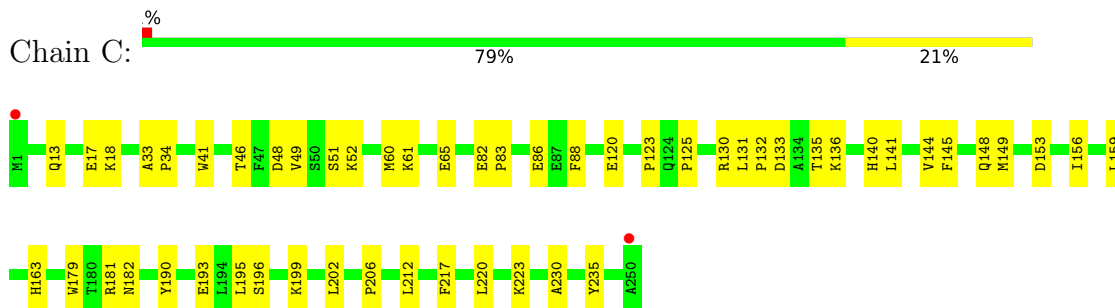
- Molecule 1: Cytosolic ascorbate peroxidase



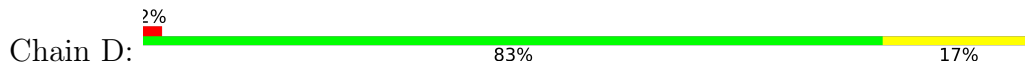
- Molecule 1: Cytosolic ascorbate peroxidase

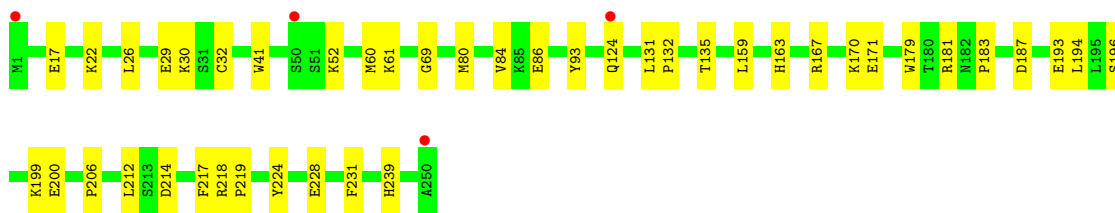


- Molecule 1: Cytosolic ascorbate peroxidase

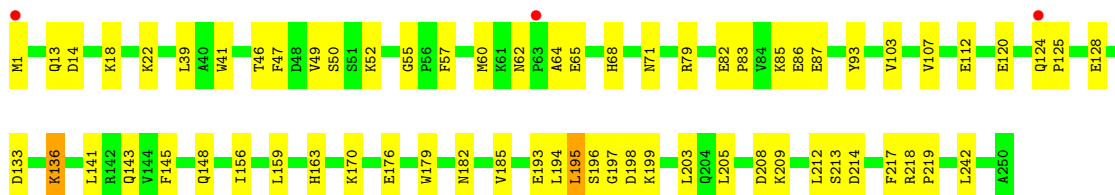


- Molecule 1: Cytosolic ascorbate peroxidase

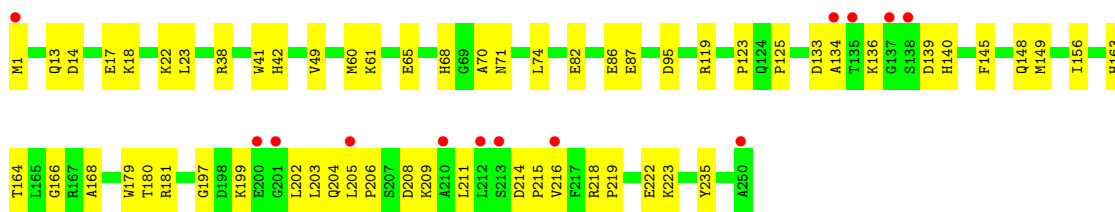
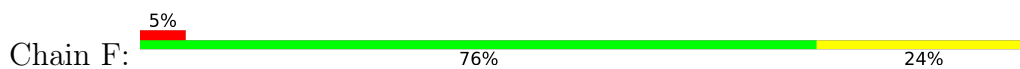




- Molecule 1: Cytosolic ascorbate peroxidase



- Molecule 1: Cytosolic ascorbate peroxidase



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 97.1 (49.23-2.19)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.20	Depositor
R, $R_{free}$	0.188 , 0.242 0.188 , 0.242	Depositor DCC
$R_{free}$ test set	1993 reflections (2.34%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.3	Xtrriage
Anisotropy	0.486	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 29.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.009 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13011	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.38	0/1971	0.53	0/2668
1	B	0.34	0/1971	0.51	0/2668
1	C	0.33	0/1971	0.47	0/2668
1	D	0.37	0/1971	0.52	0/2668
1	E	0.33	0/1971	0.47	0/2668
1	F	0.33	0/1971	0.48	0/2668
All	All	0.35	0/11826	0.50	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	43	0
1	B	1923	0	1884	64	0
1	C	1923	0	1884	38	0
1	D	1923	0	1885	36	0
1	E	1923	0	1884	54	0
1	F	1923	0	1885	56	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	8	0
5	E	135	0	0	6	0
5	F	124	0	0	7	0
All	All	12783	228	11534	299	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 13.

All (299) 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	1.37	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:36:MET:HE3	1:B:36:MET:HA	1.64	0.77
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: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: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
1:F:65:GLU:HA	1:F:68:HIS:CE1	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:MET:HE1	1:E:71:ASN:ND2	2.13	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:48:ASP:OD2	1:C:51:SER:OG	2.14	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: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: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:193:GLU:OE1	1:E:199:LYS:NZ	2.37	0.57
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:36:MET:HE1	1:B:39:LEU:HD23	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:B:36:MET:HE3	1:B:36:MET:CA	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:82:GLU:O	1:E:86:GLU:HG3	2.08	0.54
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:B:1:MET:HE2	1:B:1:MET:HA	1.89	0.53
1:C:145:PHE:HA	1:C:149:MET:HE3	1.89	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: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:B:36:MET:HE1	1:B:81:LEU:HD11	1.92	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:A:57:PHE:C	1:A:94:ALA:HB2	2.34	0.52
1:B:141:LEU:HD22	3:B:302:HEM:HBB1	1.91	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:D:30:LYS:HD2	1:D:80:MET:HE3	1.93	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:A:124:GLN:HA	1:A:124:GLN:OE1	2.09	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:B:86:GLU:CD	1:E:79:ARG:HE	2.19	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:E:163:HIS:HB3	1:E:179:TRP:CD2	2.47	0.49
1:F:223:LYS:NZ	5:F:404:HOH:O	2.23	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:B:36:MET:HE2	1:B:81:LEU:HD11	1.94	0.48
1:D:135:THR:HA	1:D:206:PRO:HG2	1.95	0.48
1:B:36:MET:HE1	1:B:39:LEU:CD2	2.43	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:C:41:TRP:CH2	1:C:149:MET:HE1	2.50	0.47
1:C:235:TYR:C	1:C:235:TYR:CD1	2.93	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: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:B:36:MET:HA	1:B:36:MET:CE	2.41	0.46
1:D:61:LYS:HD3	1:D:93:TYR:CZ	2.51	0.46
1:F:209:LYS:C	1:F:211:LEU:N	2.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:26:LEU:C	1:D:26:LEU:HD23	2.41	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: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
1:B:36:MET:HE2	1:B:100:ALA:HB1	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:133:ASP:CG	1:F:136:LYS:HD2	2.42	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
1:F:215:PRO:O	1:F:219:PRO:CD	2.66	0.43
1:D:187:ASP:OD1	1:D:187:ASP:C	2.62	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:F:209:LYS:C	1:F:211:LEU:H	2.26	0.43
1:F:41:TRP:CZ3	1:F:149:MET:HE1	2.54	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:D:124:GLN:H	1:D:124:GLN:CD	2.26	0.42
1:E:141:LEU:HD22	3:E:302:HEM:CBB	2.43	0.42
1:F:235:TYR:CD1	1:F:235:TYR:C	2.97	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: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:60:MET:HE2	1:A:60:MET:HB2	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:182:ASN:OD1	1:C:182:ASN:N	2.53	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:C:145:PHE:CD2	1:C:149:MET:HE3	2.55	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:C:60:MET:HE2	1:C:60:MET:HB2	1.89	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
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:A:145:PHE:CA	1:A:149:MET:HE3	2.27	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:E:46:THR:OG1	5:E:402:HOH:O	2.10	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:LYS:HE3	1:E:93:TYR:CE2	2.56	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%)	197 (98%)	3 (2%)	57	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	200/200 (100%)	194 (97%)	6 (3%)	36	49
1	C	200/200 (100%)	198 (99%)	2 (1%)	68	81
1	D	200/200 (100%)	198 (99%)	2 (1%)	68	81
1	E	200/200 (100%)	197 (98%)	3 (2%)	57	73
1	F	200/200 (100%)	199 (100%)	1 (0%)	81	90
All	All	1200/1200 (100%)	1183 (99%)	17 (1%)	59	75

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	41	TRP
1	A	195	LEU
1	B	41	TRP
1	B	50	SER
1	B	120	GLU
1	B	199	LYS
1	B	216	VAL
1	B	223	LYS
1	C	13	GLN
1	C	120	GLU
1	D	41	TRP
1	D	196	SER
1	E	50	SER
1	E	136	LYS
1	E	195	LEU
1	F	139	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	148	GLN
1	E	62	ASN
1	E	98	GLN
1	F	13	GLN

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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
2	ASC	C	301	-	12,12,12	3.05	6 (50%)	17,17,17	2.22	6 (35%)
2	ASC	B	301	-	12,12,12	2.86	5 (41%)	17,17,17	2.42	8 (47%)
2	ASC	E	301	-	12,12,12	2.99	4 (33%)	17,17,17	2.08	5 (29%)
3	HEM	A	302	5,1	50,50,50	1.50	9 (18%)	67,82,82	1.11	6 (8%)
3	HEM	F	302	5,1	50,50,50	1.42	7 (14%)	67,82,82	1.20	5 (7%)
3	HEM	B	302	5,1	50,50,50	1.65	8 (16%)	67,82,82	1.00	0
3	HEM	E	302	5,1	50,50,50	1.50	7 (14%)	67,82,82	1.13	5 (7%)
2	ASC	D	301	-	12,12,12	2.90	5 (41%)	17,17,17	2.32	6 (35%)
3	HEM	D	302	5,1	50,50,50	1.56	10 (20%)	67,82,82	1.24	6 (8%)
3	HEM	C	302	5,1	50,50,50	1.42	7 (14%)	67,82,82	1.10	2 (2%)
2	ASC	F	301	-	12,12,12	2.70	4 (33%)	17,17,17	2.78	9 (52%)
2	ASC	A	301	-	12,12,12	2.81	5 (41%)	17,17,17	2.36	4 (23%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ASC	C	301	-	-	2/6/22/22	0/1/1/1
2	ASC	B	301	-	-	3/6/22/22	0/1/1/1
2	ASC	E	301	-	-	2/6/22/22	0/1/1/1
3	HEM	A	302	5,1	-	5/14/54/54	-
3	HEM	F	302	5,1	-	2/14/54/54	-
3	HEM	B	302	5,1	-	2/14/54/54	-
3	HEM	E	302	5,1	-	2/14/54/54	-
2	ASC	D	301	-	-	0/6/22/22	0/1/1/1
3	HEM	D	302	5,1	-	2/14/54/54	-
3	HEM	C	302	5,1	-	6/14/54/54	-
2	ASC	F	301	-	-	6/6/22/22	0/1/1/1
2	ASC	A	301	-	-	0/6/22/22	0/1/1/1

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	ASC	O4-C1	8.52	1.49	1.36
2	E	301	ASC	O4-C1	8.36	1.49	1.36
2	D	301	ASC	O4-C1	8.22	1.49	1.36
2	B	301	ASC	O4-C1	8.03	1.49	1.36
2	A	301	ASC	O4-C1	7.81	1.48	1.36
2	F	301	ASC	O4-C1	7.54	1.48	1.36
3	B	302	HEM	FE-ND	6.20	2.14	1.94
3	B	302	HEM	FE-NA	4.89	2.11	1.95
3	C	302	HEM	FE-ND	4.74	2.09	1.94
3	E	302	HEM	FE-ND	4.59	2.09	1.94
3	D	302	HEM	FE-ND	4.47	2.08	1.94
3	D	302	HEM	FE-NB	4.16	2.07	1.94
3	F	302	HEM	FE-ND	4.01	2.07	1.94
3	E	302	HEM	FE-NA	3.84	2.07	1.95
2	C	301	ASC	O4-C4	3.49	1.51	1.45
3	C	302	HEM	FE-NC	3.45	2.06	1.95
2	E	301	ASC	O4-C4	3.43	1.51	1.45
3	D	302	HEM	FE-NA	3.40	2.06	1.95
3	E	302	HEM	FE-NC	3.38	2.06	1.95
3	A	302	HEM	FE-ND	3.35	2.05	1.94
3	F	302	HEM	FE-NB	3.30	2.05	1.94
3	A	302	HEM	FE-NA	3.30	2.06	1.95
3	A	302	HEM	FE-NC	3.28	2.06	1.95
2	D	301	ASC	O4-C4	3.16	1.51	1.45
3	F	302	HEM	CAC-C3C	3.04	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	HEM	CAB-C3B	3.02	1.55	1.47
3	C	302	HEM	CAB-C3B	2.92	1.55	1.47
3	E	302	HEM	CAB-C3B	2.89	1.55	1.47
3	D	302	HEM	CAB-C3B	2.87	1.55	1.47
2	F	301	ASC	O4-C4	2.85	1.50	1.45
3	B	302	HEM	CAB-C3B	2.84	1.55	1.47
3	A	302	HEM	CAC-C3C	2.82	1.54	1.47
3	D	302	HEM	CAC-C3C	2.81	1.54	1.47
2	C	301	ASC	C5-C4	-2.77	1.48	1.53
2	B	301	ASC	O4-C4	2.77	1.50	1.45
3	F	302	HEM	CAB-C3B	2.72	1.54	1.47
2	F	301	ASC	O3-C3	2.70	1.42	1.32
3	B	302	HEM	CAC-C3C	2.68	1.54	1.47
3	C	302	HEM	CAC-C3C	2.66	1.54	1.47
2	A	301	ASC	O4-C4	2.63	1.50	1.45
3	E	302	HEM	CAC-C3C	2.59	1.54	1.47
2	A	301	ASC	O3-C3	2.54	1.41	1.32
2	A	301	ASC	C5-C4	-2.52	1.48	1.53
2	B	301	ASC	O3-C3	2.51	1.41	1.32
3	D	302	HEM	FE-NC	2.50	2.03	1.95
2	E	301	ASC	O3-C3	2.45	1.41	1.32
2	B	301	ASC	O2-C2	2.43	1.41	1.33
2	D	301	ASC	O3-C3	2.42	1.41	1.32
3	A	302	HEM	FE-NB	2.39	2.02	1.94
2	C	301	ASC	O3-C3	2.38	1.41	1.32
2	B	301	ASC	C5-C4	-2.38	1.48	1.53
2	E	301	ASC	C5-C4	-2.36	1.48	1.53
3	D	302	HEM	CMA-C3A	2.32	1.55	1.50
2	C	301	ASC	O2-C2	2.27	1.41	1.33
3	A	302	HEM	CMA-C3A	2.23	1.55	1.50
3	B	302	HEM	CMD-C2D	2.23	1.55	1.50
3	F	302	HEM	FE-NA	2.21	2.02	1.95
2	D	301	ASC	C5-C4	-2.20	1.49	1.53
3	E	302	HEM	CMA-C3A	2.18	1.55	1.50
3	D	302	HEM	CMD-C2D	2.18	1.55	1.50
2	F	301	ASC	O2-C2	2.18	1.41	1.33
3	F	302	HEM	FE-NC	2.18	2.02	1.95
2	A	301	ASC	C4-C3	-2.16	1.46	1.50
3	A	302	HEM	CMB-C2B	2.15	1.55	1.50
3	C	302	HEM	CMC-C2C	2.15	1.55	1.50
2	D	301	ASC	O2-C2	2.13	1.40	1.33
2	C	301	ASC	C4-C3	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	HEM	CMC-C2C	2.12	1.55	1.50
3	C	302	HEM	CMB-C2B	2.11	1.55	1.50
3	B	302	HEM	FE-NC	2.10	2.02	1.95
3	F	302	HEM	CMD-C2D	2.09	1.55	1.50
3	B	302	HEM	CMB-C2B	2.08	1.55	1.50
3	C	302	HEM	C2A-C3A	-2.07	1.33	1.38
3	E	302	HEM	CMB-C2B	2.03	1.54	1.50
3	D	302	HEM	CMB-C2B	2.02	1.54	1.50
3	A	302	HEM	C3D-C2D	-2.01	1.32	1.36
3	B	302	HEM	CAD-C3D	2.00	1.56	1.51

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	ASC	O4-C1-C2	-5.72	104.80	109.86
2	F	301	ASC	O4-C1-C2	-5.33	105.14	109.86
2	C	301	ASC	O4-C1-C2	-5.22	105.24	109.86
2	D	301	ASC	O4-C1-C2	-5.03	105.41	109.86
2	D	301	ASC	O4-C1-O1	5.02	127.89	121.27
2	F	301	ASC	O3-C3-C2	-4.89	119.89	132.40
2	B	301	ASC	O4-C1-C2	-4.56	105.82	109.86
2	E	301	ASC	O4-C1-C2	-4.52	105.86	109.86
2	B	301	ASC	O3-C3-C2	-4.33	121.31	132.40
2	A	301	ASC	O4-C1-O1	4.27	126.89	121.27
2	F	301	ASC	O4-C1-O1	4.23	126.85	121.27
2	C	301	ASC	O4-C1-O1	3.96	126.49	121.27
2	A	301	ASC	O3-C3-C2	-3.90	122.42	132.40
2	A	301	ASC	C5-C4-C3	-3.78	107.77	114.71
2	F	301	ASC	C1-C2-C3	3.69	112.30	107.77
3	E	302	HEM	CHC-C4B-NB	3.66	128.36	124.42
2	E	301	ASC	O4-C1-O1	3.60	126.02	121.27
2	B	301	ASC	O5-C5-C4	3.56	117.48	110.74
2	B	301	ASC	O4-C1-O1	3.39	125.74	121.27
2	E	301	ASC	O3-C3-C2	-3.33	123.87	132.40
2	D	301	ASC	C5-C4-C3	-3.22	108.80	114.71
2	D	301	ASC	O3-C3-C2	-3.19	124.23	132.40
2	B	301	ASC	C6-C5-C4	-3.12	106.61	111.86
2	E	301	ASC	C6-C5-C4	-3.05	106.72	111.86
3	F	302	HEM	C3B-C4B-NB	-3.00	107.31	109.47
2	F	301	ASC	C5-C4-C3	-2.98	109.25	114.71
2	B	301	ASC	C4-O4-C1	-2.91	106.09	109.27
2	F	301	ASC	O5-C5-C4	2.87	116.19	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	ASC	C6-C5-C4	-2.84	107.07	111.86
3	C	302	HEM	CAA-CBA-CGA	-2.82	106.19	113.67
3	D	302	HEM	C3B-C4B-NB	-2.75	107.49	109.47
2	C	301	ASC	O3-C3-C2	-2.68	125.54	132.40
3	D	302	HEM	C2A-C1A-NA	-2.65	107.21	110.15
3	D	302	HEM	C1B-NB-C4B	2.64	108.33	105.21
2	C	301	ASC	C1-C2-C3	2.60	110.96	107.77
3	F	302	HEM	C3B-C2B-C1B	2.57	108.34	106.41
3	A	302	HEM	CAA-CBA-CGA	-2.50	107.02	113.67
2	C	301	ASC	C5-C4-C3	-2.50	110.13	114.71
2	C	301	ASC	C6-C5-C4	-2.46	107.72	111.86
2	E	301	ASC	O2-C2-C3	-2.45	121.13	128.64
3	A	302	HEM	CHC-C4B-NB	2.44	127.05	124.42
3	C	302	HEM	C2A-C1A-NA	-2.43	107.45	110.15
3	E	302	HEM	C4D-ND-C1D	2.42	108.07	105.21
3	A	302	HEM	CAD-C3D-C4D	2.38	128.85	124.70
2	F	301	ASC	O3-C3-C4	2.38	124.04	117.99
3	E	302	HEM	C2A-C1A-NA	-2.37	107.52	110.15
2	B	301	ASC	O2-C2-C3	-2.36	121.41	128.64
3	F	302	HEM	C1B-NB-C4B	2.36	108.00	105.21
3	A	302	HEM	CAD-CBD-CGD	-2.33	107.48	113.67
2	D	301	ASC	O3-C3-C4	2.31	123.87	117.99
3	D	302	HEM	C4D-ND-C1D	2.25	107.87	105.21
2	B	301	ASC	C5-C4-C3	-2.22	110.64	114.71
3	E	302	HEM	C1D-C2D-C3D	2.17	109.26	106.98
3	A	302	HEM	O1D-CGD-CBD	-2.16	116.23	123.09
2	F	301	ASC	C4-O4-C1	-2.15	106.91	109.27
3	D	302	HEM	C3B-C2B-C1B	2.14	108.02	106.41
3	D	302	HEM	O2D-CGD-CBD	2.14	120.75	114.00
2	D	301	ASC	O2-C2-C3	-2.09	122.23	128.64
3	F	302	HEM	C4D-ND-C1D	2.08	107.67	105.21
3	A	302	HEM	CHD-C1D-ND	2.07	126.65	124.42
3	E	302	HEM	C2D-C1D-ND	-2.03	107.55	109.90
3	F	302	HEM	CHD-C4C-NC	2.02	126.65	124.45

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

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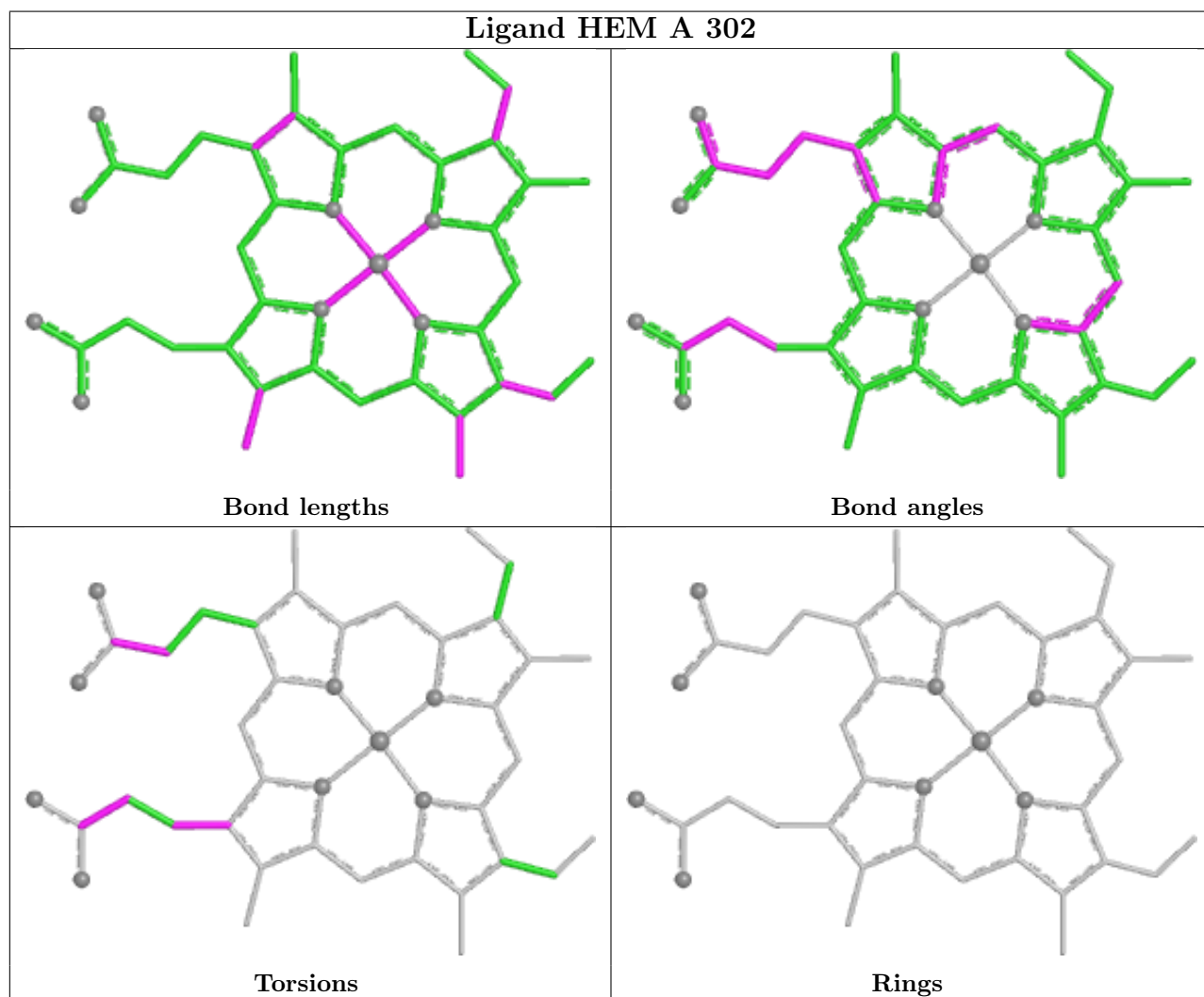
Mol	Chain	Res	Type	Atoms
2	F	301	ASC	O4-C4-C5-O5
2	F	301	ASC	C4-C5-C6-O6
2	F	301	ASC	O5-C5-C6-O6
2	B	301	ASC	O5-C5-C6-O6
2	E	301	ASC	C4-C5-C6-O6
2	C	301	ASC	C4-C5-C6-O6
2	E	301	ASC	O5-C5-C6-O6
3	C	302	HEM	C1A-C2A-CAA-CBA
2	C	301	ASC	O5-C5-C6-O6
3	A	302	HEM	C1A-C2A-CAA-CBA
2	F	301	ASC	C3-C4-C5-C6
3	F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

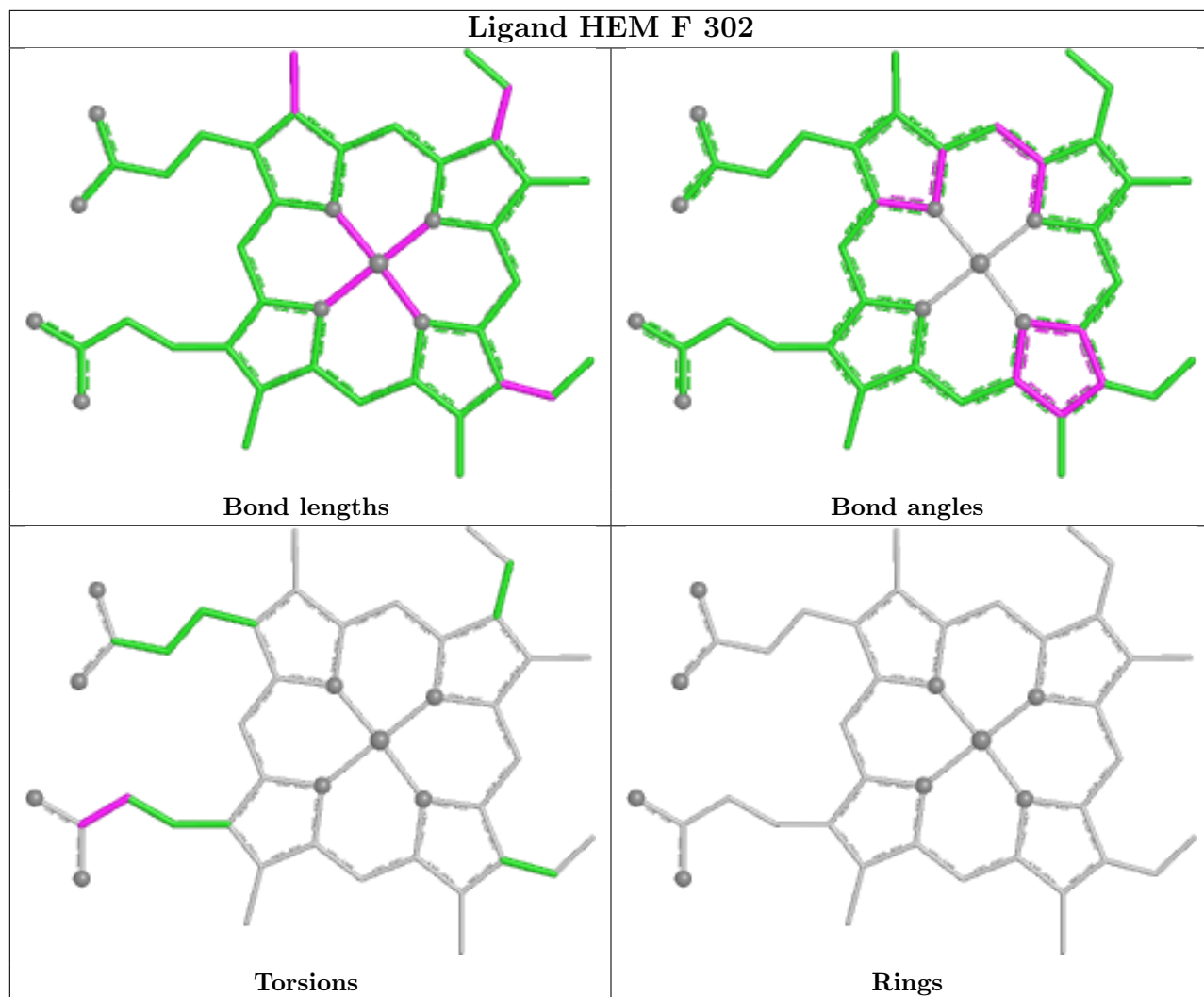
There are no ring outliers.

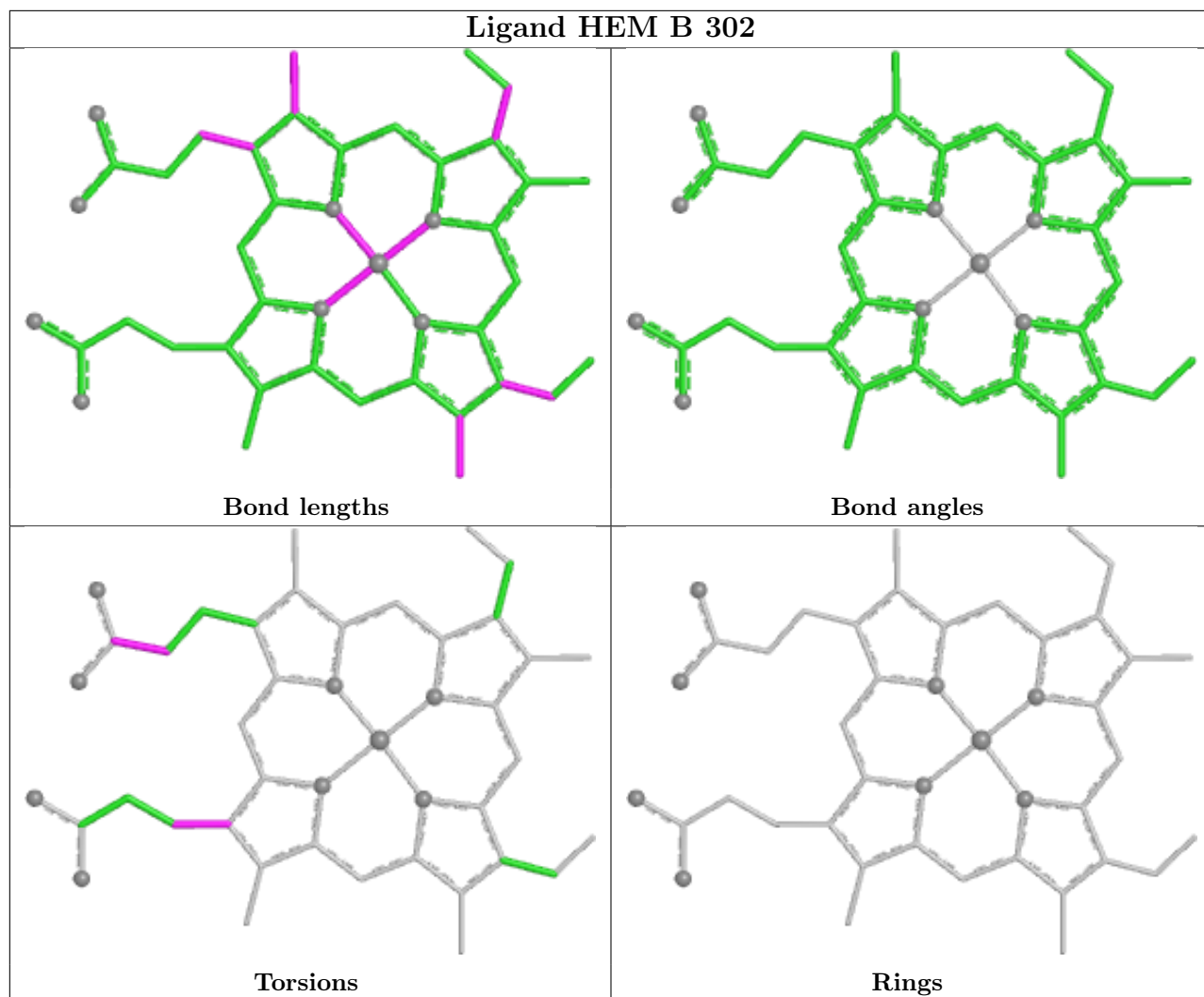
8 monomers are involved in 33 short contacts:

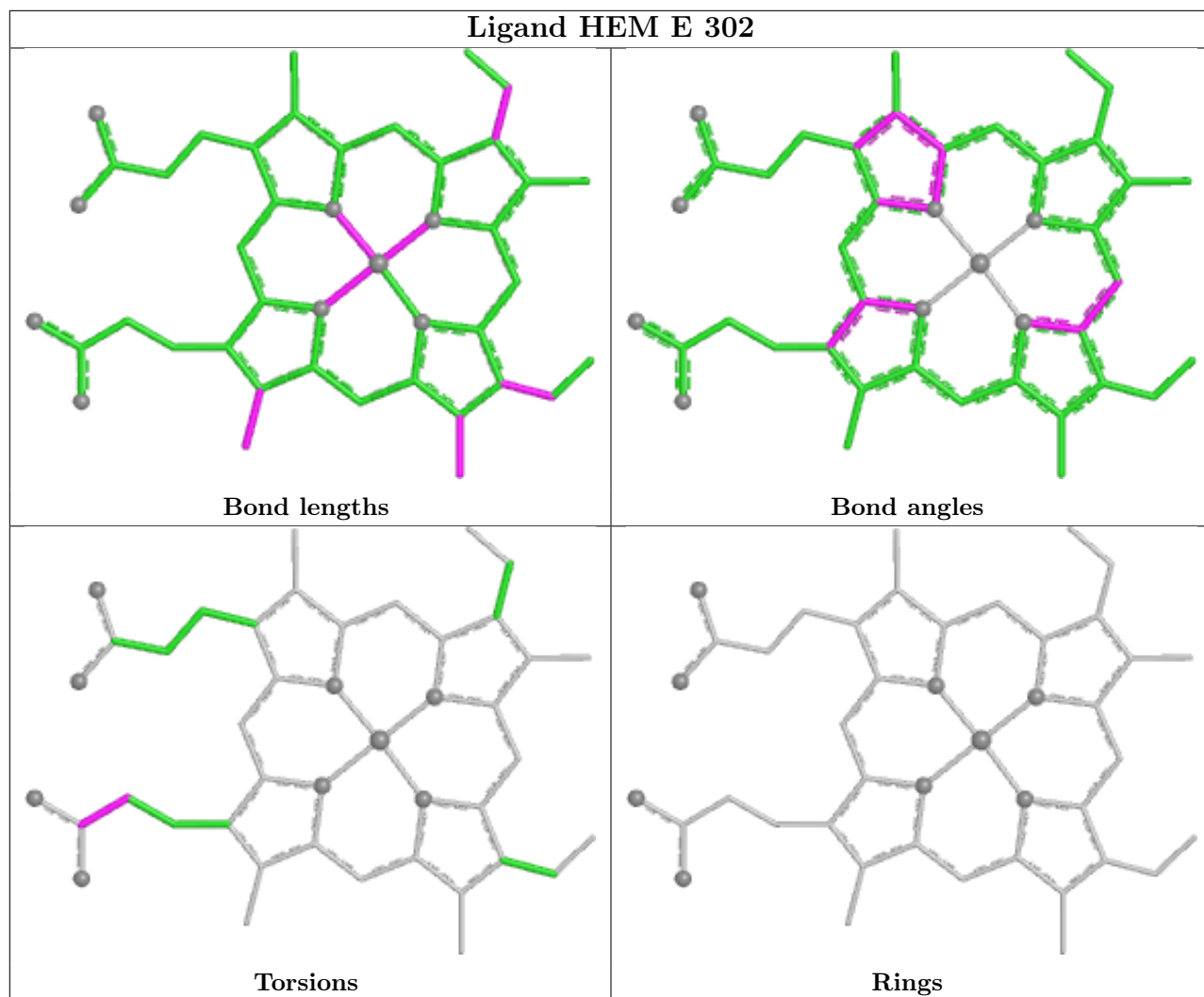
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	HEM	6	0
3	F	302	HEM	7	0
3	B	302	HEM	6	0
3	E	302	HEM	5	0
2	D	301	ASC	1	0
3	D	302	HEM	3	0
3	C	302	HEM	4	0
2	A	301	ASC	1	0

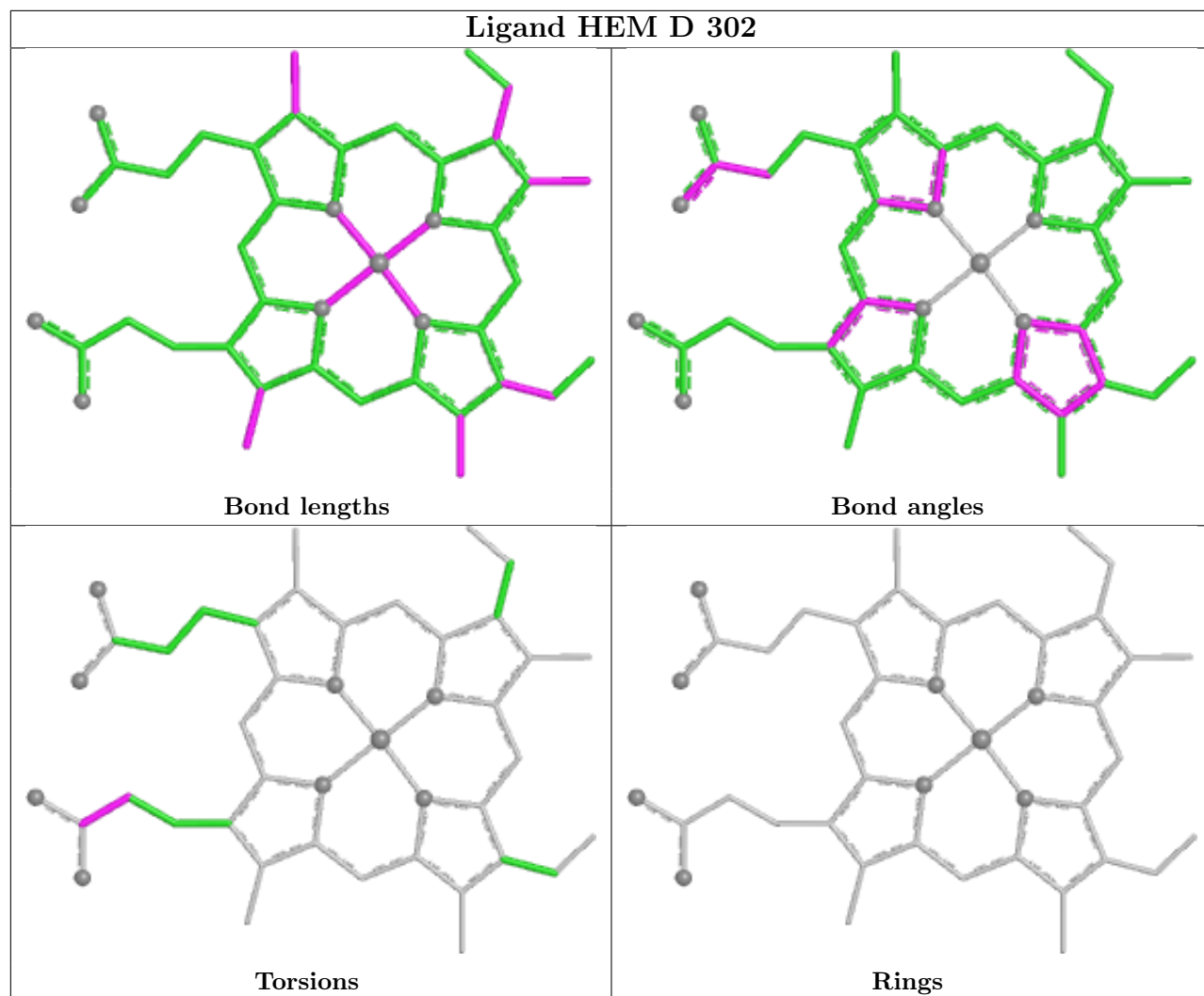
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

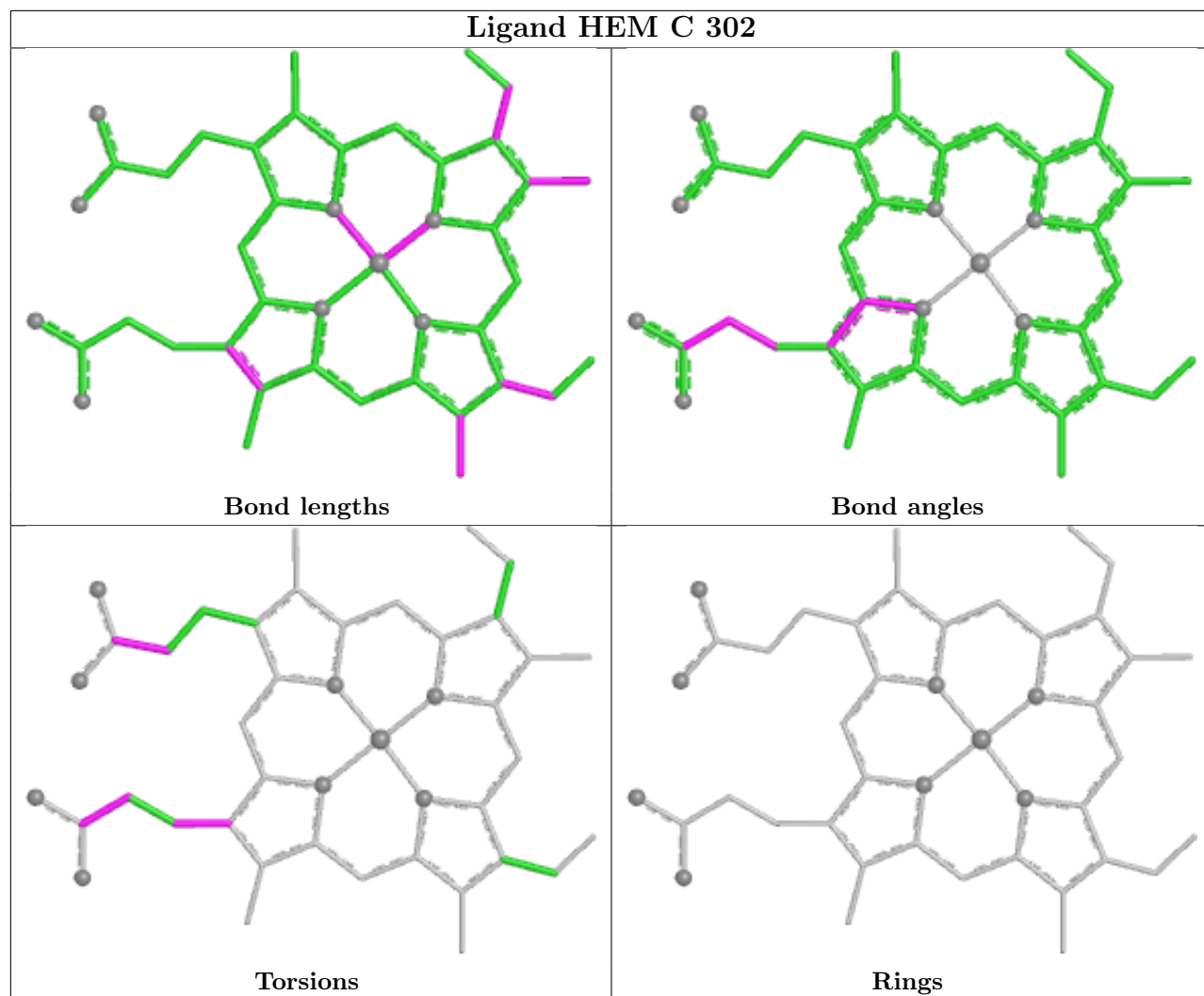












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	250/250 (100%)	-0.20	1 (0%) 88 87	18, 27, 38, 58	0
1	B	250/250 (100%)	0.02	2 (0%) 82 80	19, 32, 47, 65	0
1	C	250/250 (100%)	-0.01	2 (0%) 82 80	21, 33, 46, 57	0
1	D	250/250 (100%)	-0.16	4 (1%) 70 67	19, 28, 41, 63	0
1	E	250/250 (100%)	0.06	3 (1%) 76 74	22, 33, 47, 57	0
1	F	250/250 (100%)	0.31	13 (5%) 33 29	22, 36, 57, 76	0
All	All	1500/1500 (100%)	0.00	25 (1%) 69 66	18, 31, 49, 76	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	1	MET	4.1
1	D	250	ALA	3.4
1	A	124	GLN	3.3
1	F	200	GLU	2.9
1	F	201	GLY	2.8
1	F	137	GLY	2.7
1	F	210	ALA	2.7
1	C	250	ALA	2.7
1	F	138	SER	2.7
1	F	216	VAL	2.6
1	B	1	MET	2.5
1	F	250	ALA	2.5
1	D	50	SER	2.4
1	C	1	MET	2.4
1	D	1	MET	2.4
1	E	63	PRO	2.3
1	F	212	LEU	2.3
1	E	124	GLN	2.2
1	F	135	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	205	LEU	2.1
1	F	134	ALA	2.1
1	F	213	SER	2.1
1	B	182	ASN	2.1
1	E	1	MET	2.0
1	D	124	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

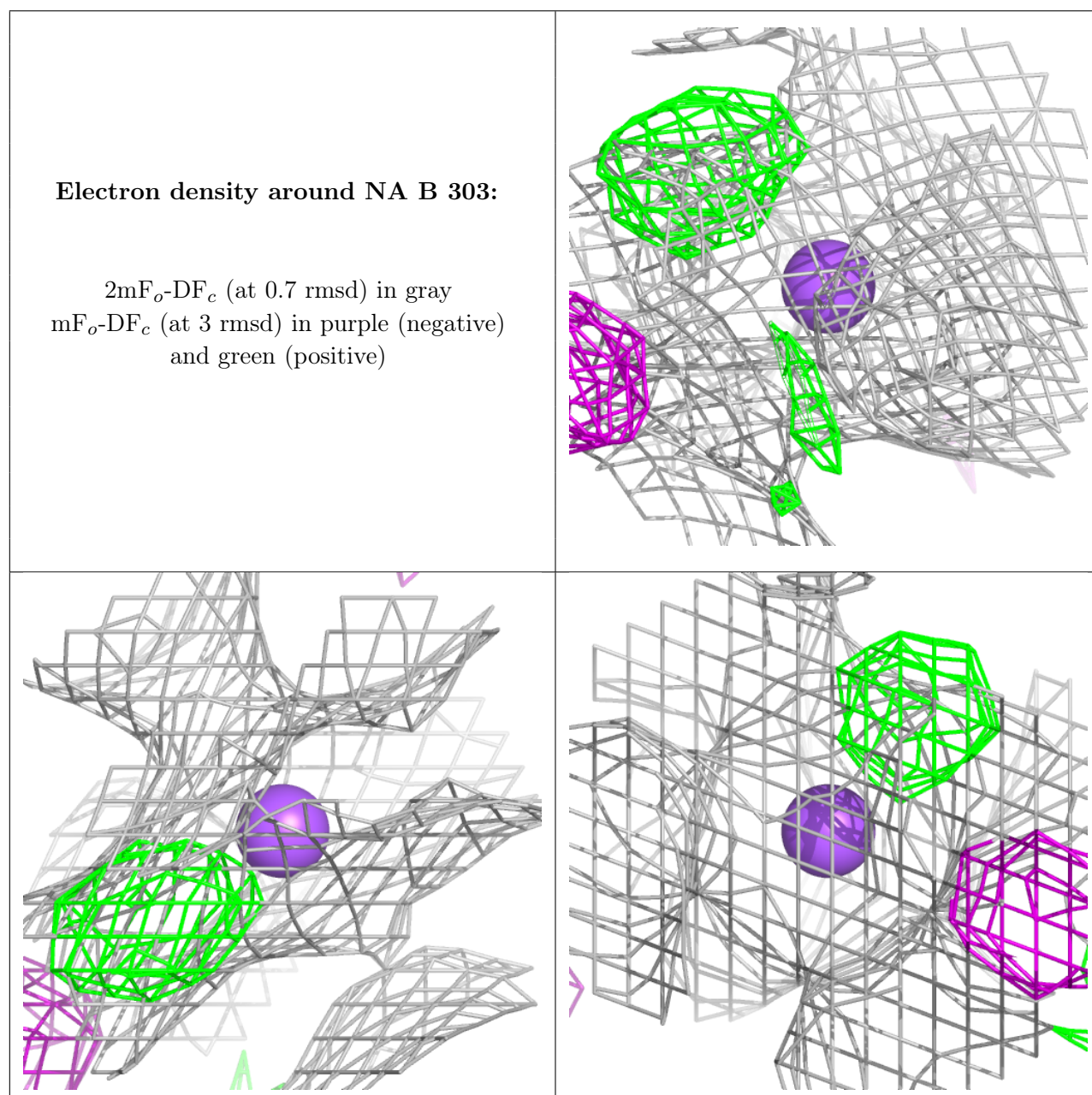
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ASC	B	301	12/12	0.90	0.09	30,37,46,48	0
2	ASC	C	301	12/12	0.90	0.08	36,45,56,58	0
2	ASC	E	301	12/12	0.90	0.09	31,39,49,53	0
2	ASC	A	301	12/12	0.91	0.08	24,35,46,54	0
2	ASC	F	301	12/12	0.91	0.08	35,44,55,55	0
2	ASC	D	301	12/12	0.92	0.07	29,37,47,56	0
4	NA	B	303	1/1	0.92	0.05	26,26,26,26	0
4	NA	D	303	1/1	0.92	0.05	25,25,25,25	0
4	NA	C	303	1/1	0.95	0.06	32,32,32,32	0
4	NA	A	303	1/1	0.95	0.05	24,24,24,24	0
4	NA	F	303	1/1	0.95	0.06	36,36,36,36	0
3	HEM	C	302	43/43	0.96	0.07	26,36,51,54	0
4	NA	E	303	1/1	0.96	0.04	30,30,30,30	0
3	HEM	B	302	43/43	0.96	0.08	25,36,53,59	0
3	HEM	E	302	43/43	0.97	0.07	24,31,39,50	0
3	HEM	F	302	43/43	0.97	0.08	30,39,51,53	0
3	HEM	A	302	43/43	0.97	0.06	19,26,37,40	0

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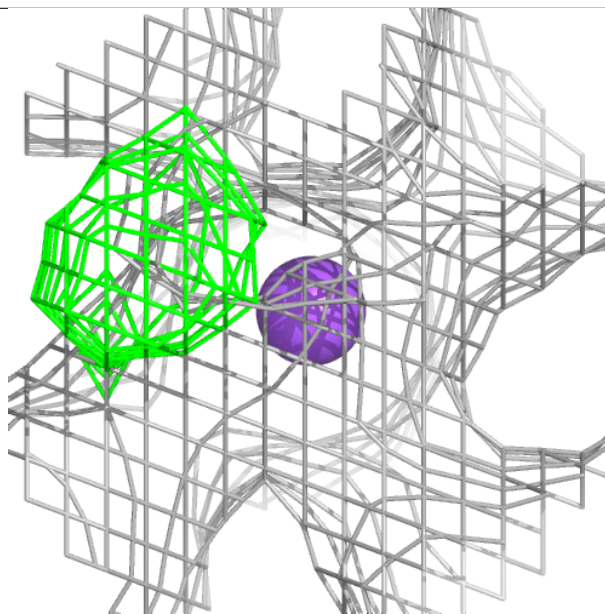
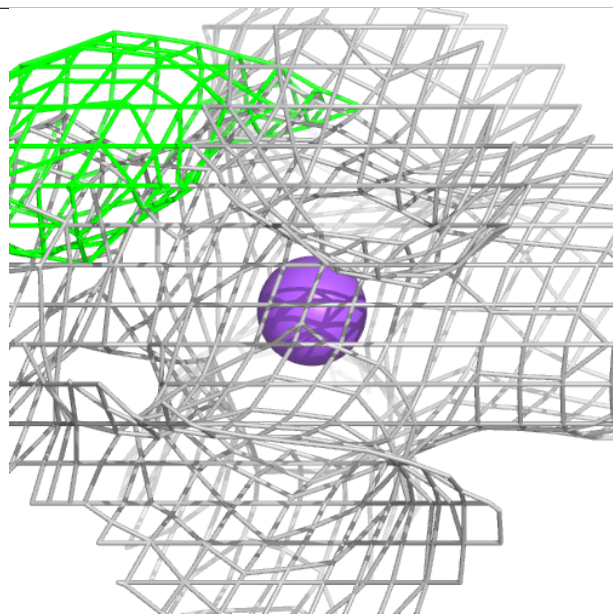
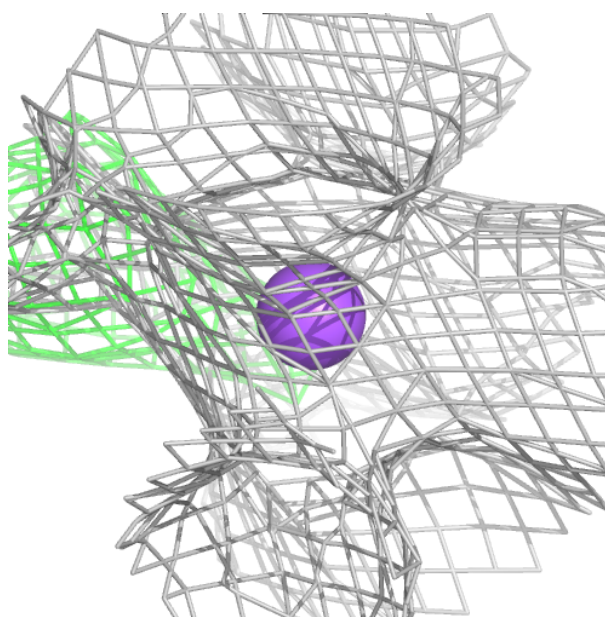
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	HEM	D	302	43/43	0.97	0.06	22,30,40,41	0

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.



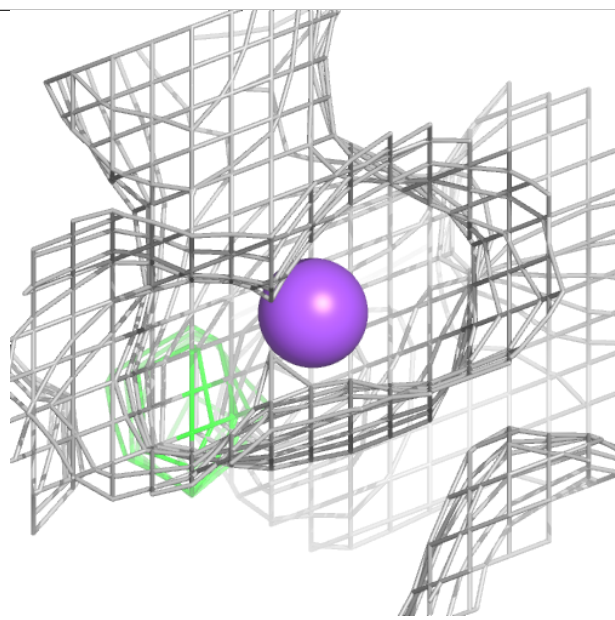
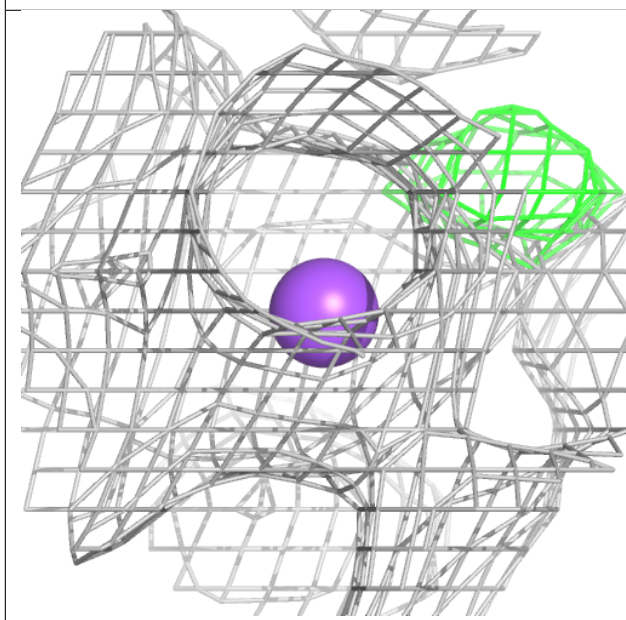
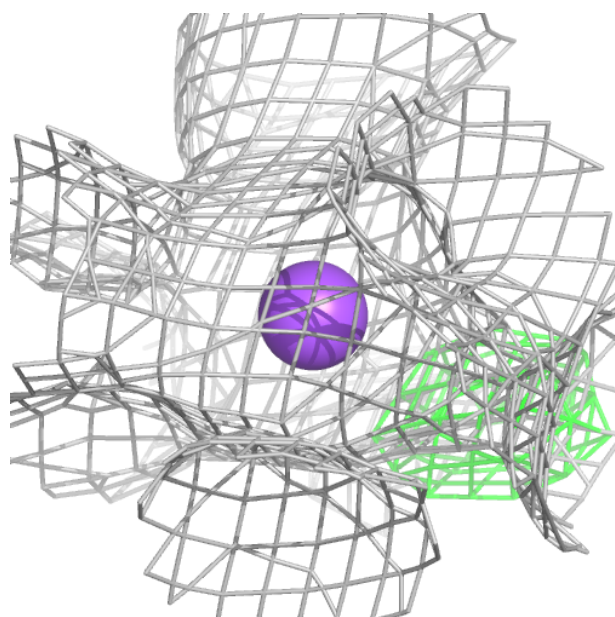
**Electron density around NA D 303:**

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



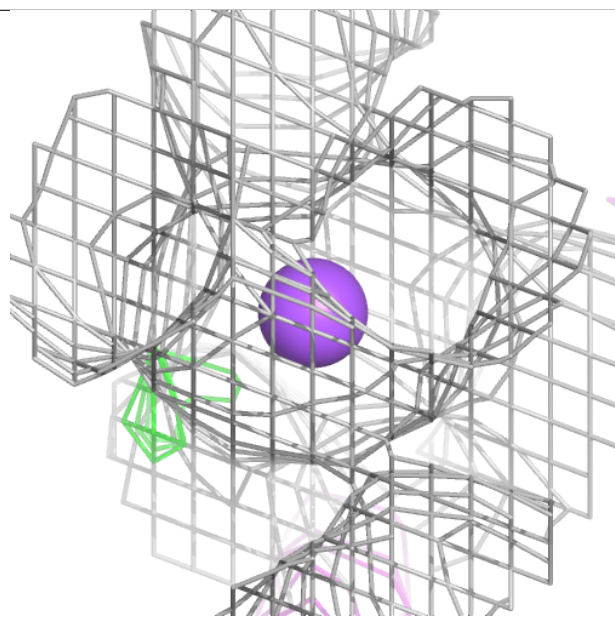
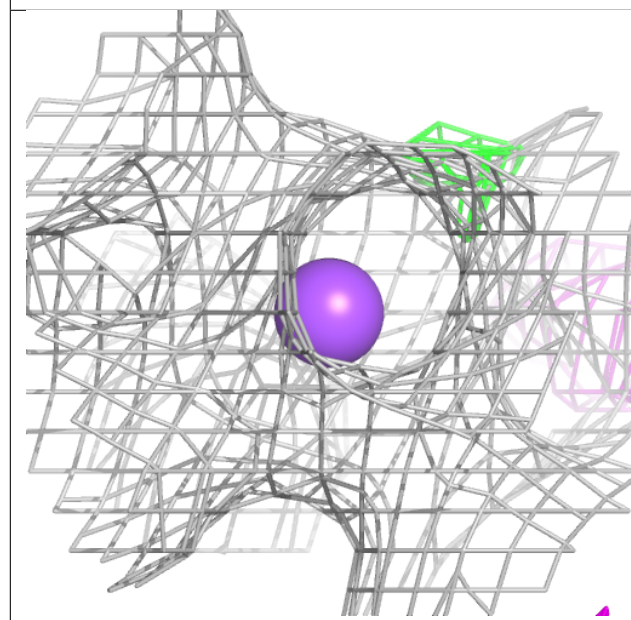
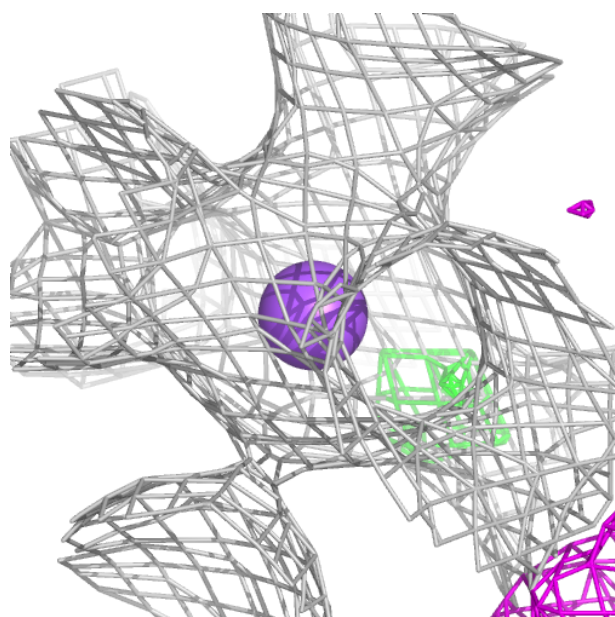
**Electron density around NA C 303:**

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



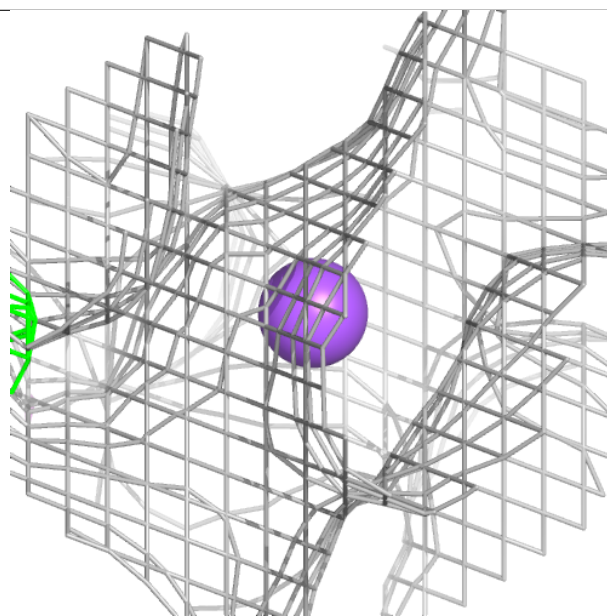
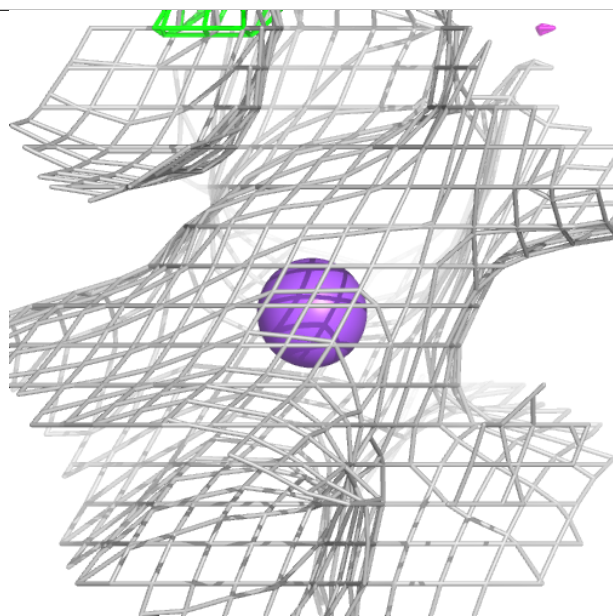
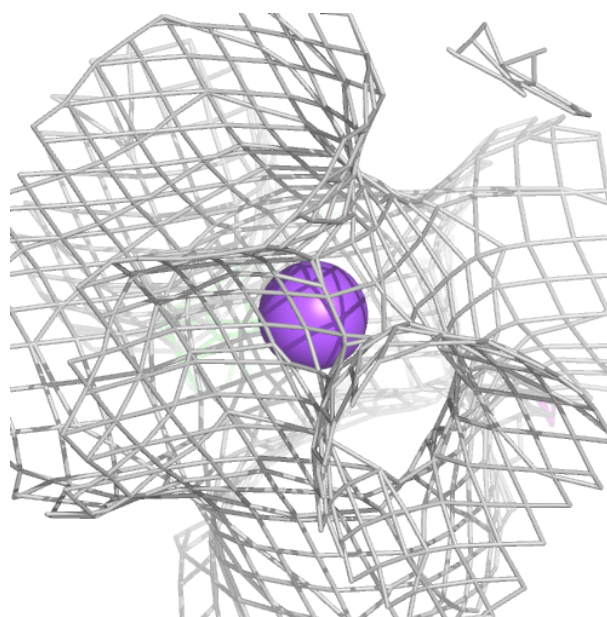
**Electron density around NA A 303:**

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



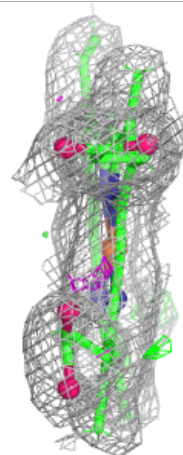
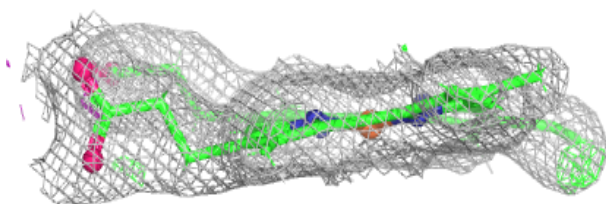
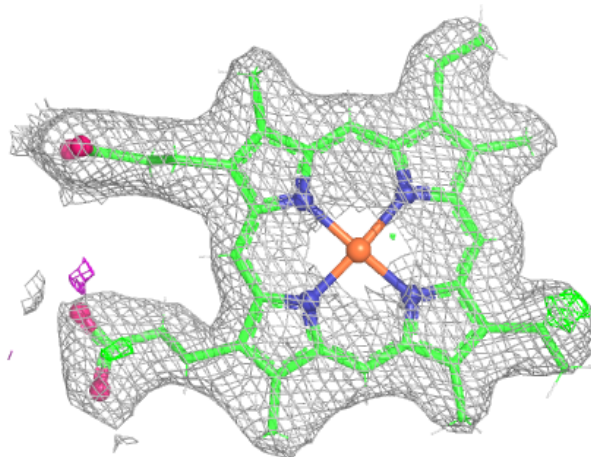
**Electron density around NA F 303:**

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



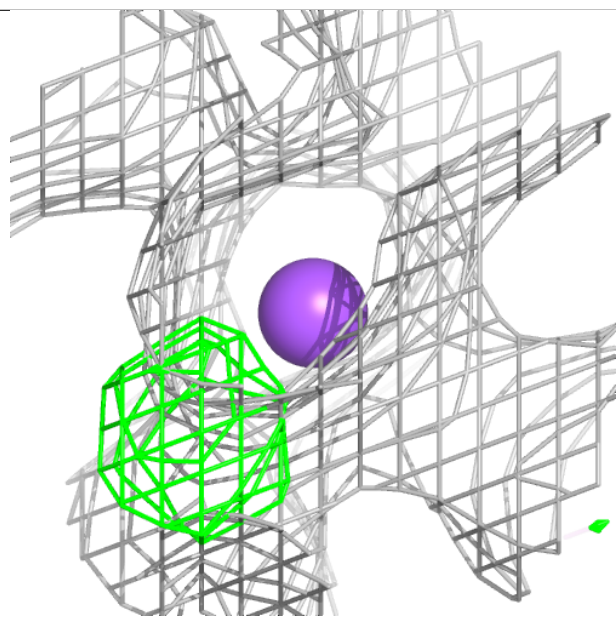
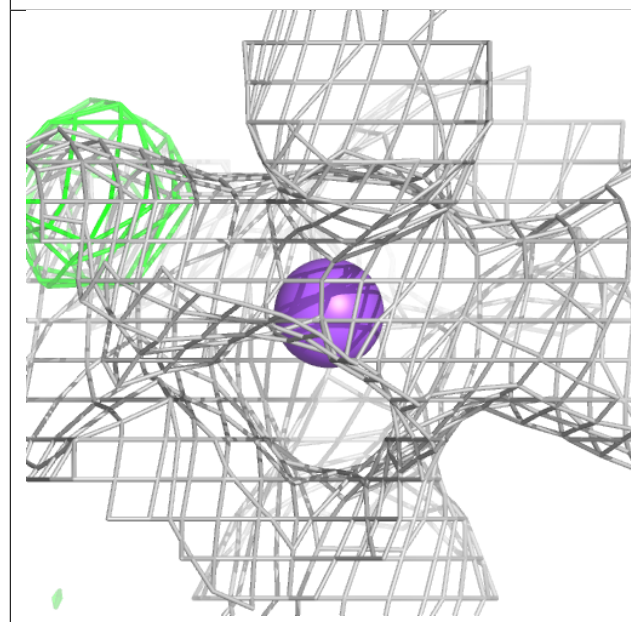
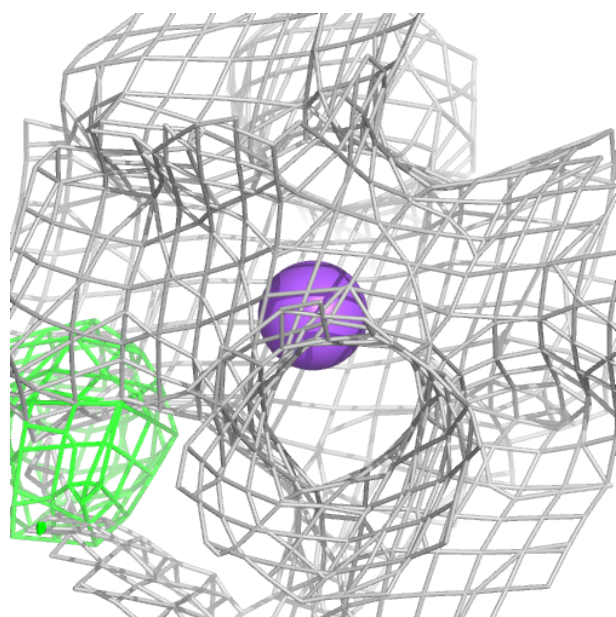
**Electron density around HEM C 302:**

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



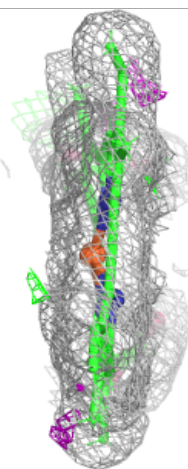
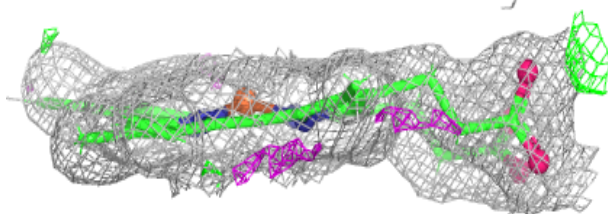
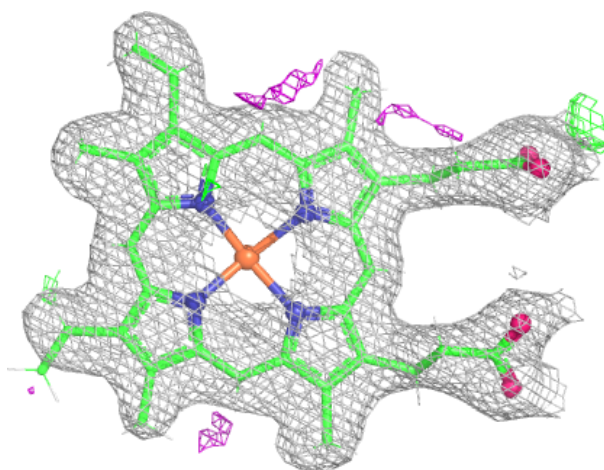
**Electron density around NA E 303:**

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



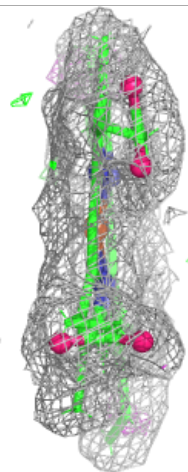
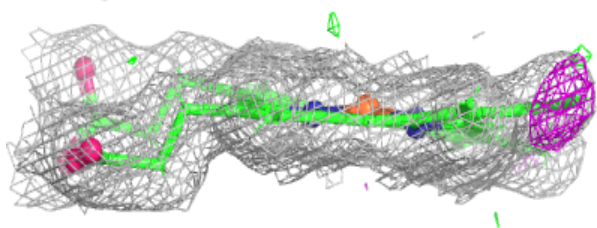
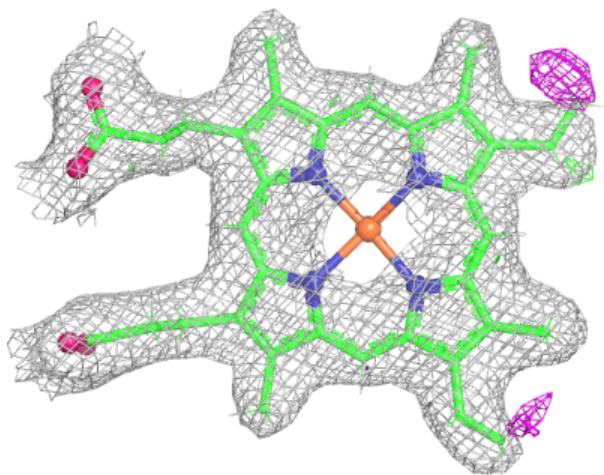
**Electron density around HEM B 302:**

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



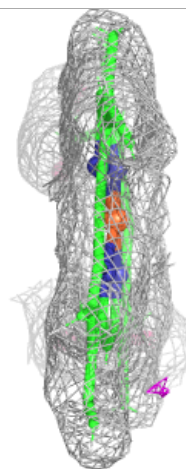
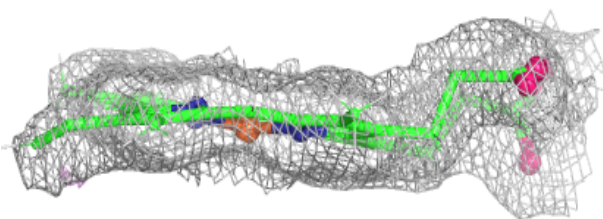
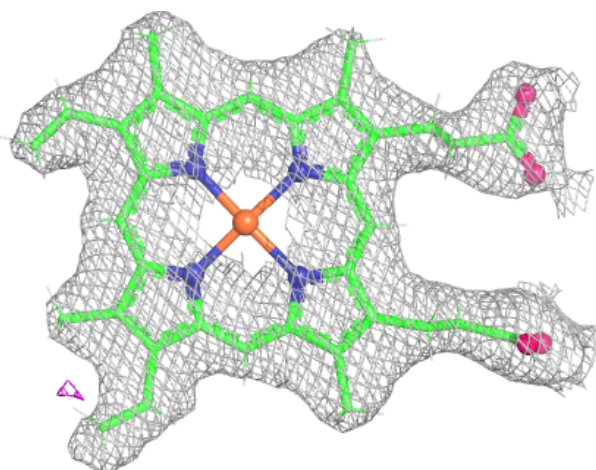
**Electron density around HEM E 302:**

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



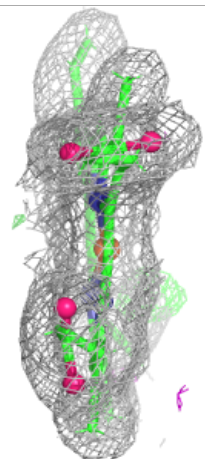
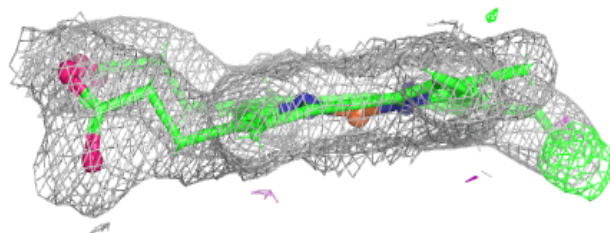
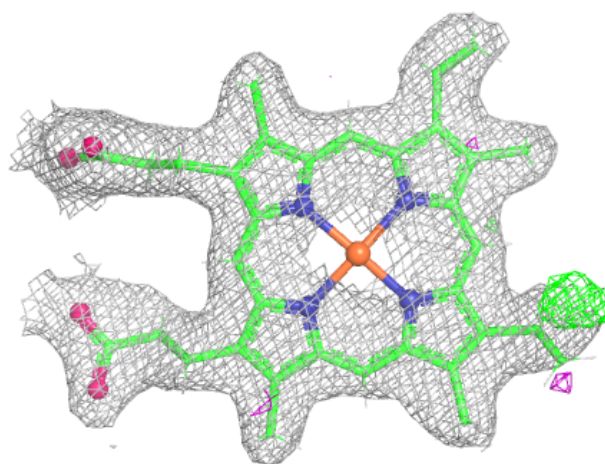
**Electron density around HEM F 302:**

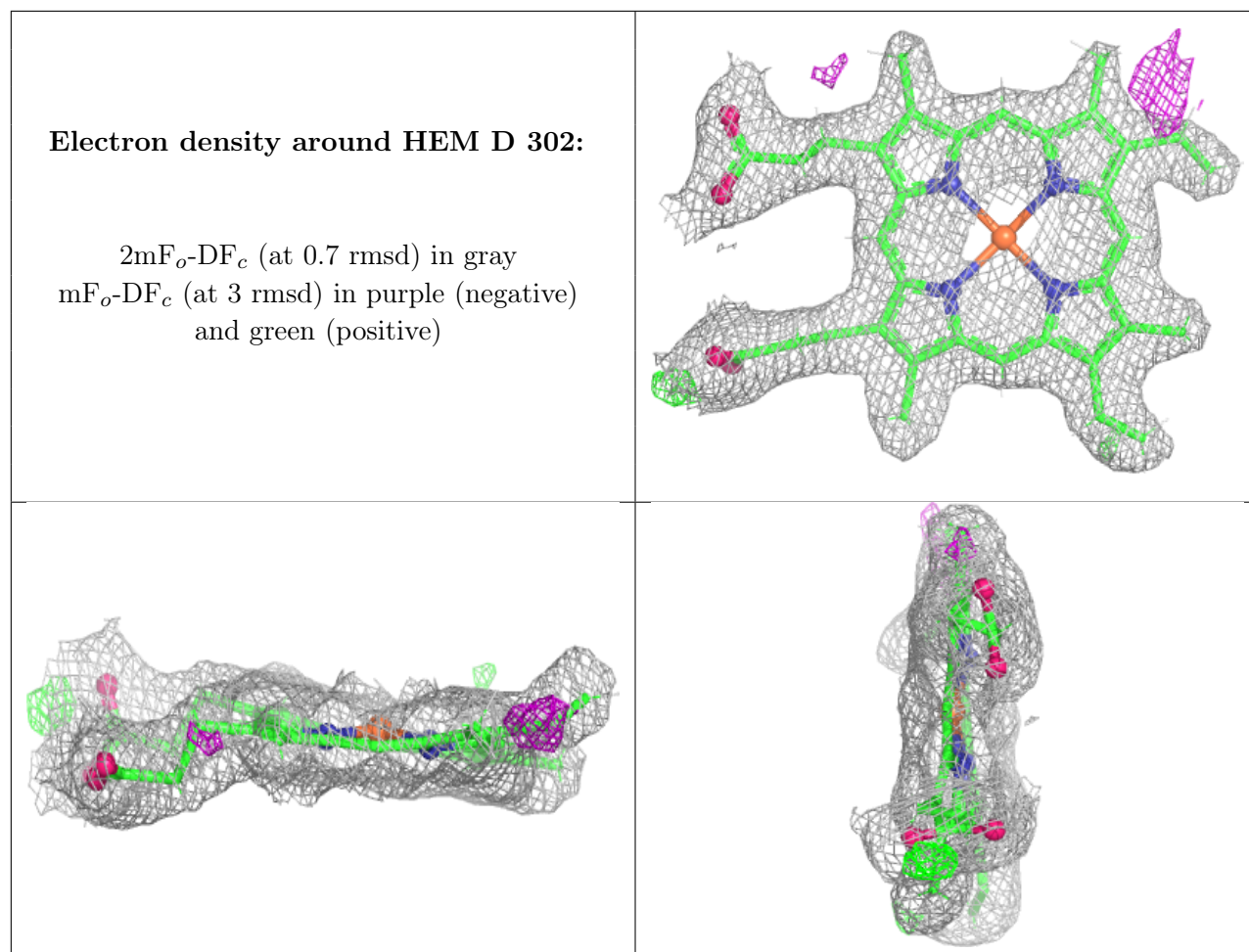
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.