



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:39 AM UTC

PDB ID : 8ED4 / pdb_00008ed4
Title : Structure of the complex between the arsenite oxidase and its native electron acceptor cytochrome c552 from Pseudorhizobium sp. str. NT-26
Authors : Maher, M.J.; Poddar, N.
Deposited on : 2022-09-03
Resolution : 2.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

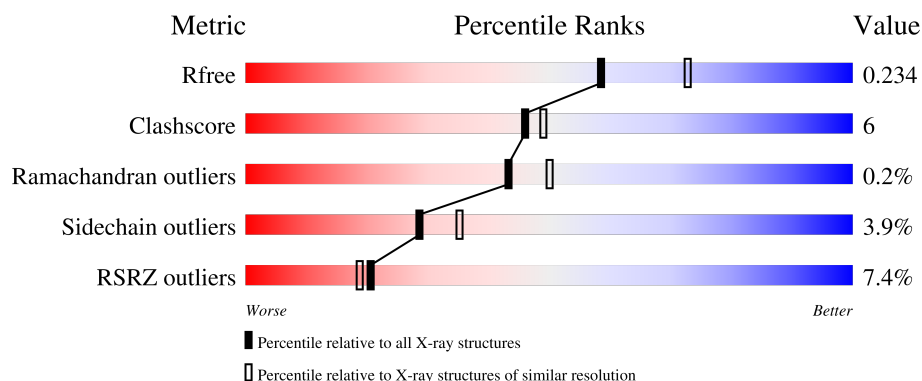
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	844	2% 88% 11% .
1	C	844	2% 87% 11% .
1	E	844	87% 11% .
1	G	844	89% 9% .
2	B	162	2% 77% . 19% .

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Mol	Chain	Length	Quality of chain
2	D	162	
2	F	162	
2	H	162	
3	I	117	
3	J	117	
3	K	117	
3	L	117	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	PG4	G	2006	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 35834 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called AroA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	843	Total	C	N	O	S	0	5	0
			6577	4110	1174	1255	38			
1	C	843	Total	C	N	O	S	0	5	0
			6573	4108	1168	1258	39			
1	E	843	Total	C	N	O	S	0	12	0
			6624	4140	1181	1265	38			
1	G	843	Total	C	N	O	S	0	9	0
			6597	4124	1175	1261	37			

- Molecule 2 is a protein called AroB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	132	Total	C	N	O	S	0	0	0
			995	629	166	198	2			
2	D	132	Total	C	N	O	S	0	0	0
			995	629	166	198	2			
2	F	132	Total	C	N	O	S	0	0	0
			995	629	166	198	2			
2	H	131	Total	C	N	O	S	0	0	0
			990	626	165	197	2			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	14	HIS	-	expression tag	UNP Q6VAL9
B	15	HIS	-	expression tag	UNP Q6VAL9
B	16	HIS	-	expression tag	UNP Q6VAL9
B	17	HIS	-	expression tag	UNP Q6VAL9
B	18	HIS	-	expression tag	UNP Q6VAL9
B	19	HIS	-	expression tag	UNP Q6VAL9
B	20	ASP	-	expression tag	UNP Q6VAL9
B	21	TYR	-	expression tag	UNP Q6VAL9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	22	ASP	-	expression tag	UNP Q6VAL9
B	23	ILE	-	expression tag	UNP Q6VAL9
B	24	PRO	-	expression tag	UNP Q6VAL9
B	25	THR	-	expression tag	UNP Q6VAL9
B	26	THR	-	expression tag	UNP Q6VAL9
B	27	GLU	-	expression tag	UNP Q6VAL9
B	28	ASN	-	expression tag	UNP Q6VAL9
B	29	LEU	-	expression tag	UNP Q6VAL9
B	30	TYR	-	expression tag	UNP Q6VAL9
B	31	PHE	-	expression tag	UNP Q6VAL9
B	32	GLN	-	expression tag	UNP Q6VAL9
B	33	GLY	-	expression tag	UNP Q6VAL9
B	34	ALA	-	expression tag	UNP Q6VAL9
B	35	MET	-	expression tag	UNP Q6VAL9
B	36	GLY	-	expression tag	UNP Q6VAL9
B	37	SER	-	expression tag	UNP Q6VAL9
B	38	GLY	-	expression tag	UNP Q6VAL9
B	39	ILE	-	expression tag	UNP Q6VAL9
B	40	GLN	-	expression tag	UNP Q6VAL9
D	14	HIS	-	expression tag	UNP Q6VAL9
D	15	HIS	-	expression tag	UNP Q6VAL9
D	16	HIS	-	expression tag	UNP Q6VAL9
D	17	HIS	-	expression tag	UNP Q6VAL9
D	18	HIS	-	expression tag	UNP Q6VAL9
D	19	HIS	-	expression tag	UNP Q6VAL9
D	20	ASP	-	expression tag	UNP Q6VAL9
D	21	TYR	-	expression tag	UNP Q6VAL9
D	22	ASP	-	expression tag	UNP Q6VAL9
D	23	ILE	-	expression tag	UNP Q6VAL9
D	24	PRO	-	expression tag	UNP Q6VAL9
D	25	THR	-	expression tag	UNP Q6VAL9
D	26	THR	-	expression tag	UNP Q6VAL9
D	27	GLU	-	expression tag	UNP Q6VAL9
D	28	ASN	-	expression tag	UNP Q6VAL9
D	29	LEU	-	expression tag	UNP Q6VAL9
D	30	TYR	-	expression tag	UNP Q6VAL9
D	31	PHE	-	expression tag	UNP Q6VAL9
D	32	GLN	-	expression tag	UNP Q6VAL9
D	33	GLY	-	expression tag	UNP Q6VAL9
D	34	ALA	-	expression tag	UNP Q6VAL9
D	35	MET	-	expression tag	UNP Q6VAL9
D	36	GLY	-	expression tag	UNP Q6VAL9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	37	SER	-	expression tag	UNP Q6VAL9
D	38	GLY	-	expression tag	UNP Q6VAL9
D	39	ILE	-	expression tag	UNP Q6VAL9
D	40	GLN	-	expression tag	UNP Q6VAL9
F	14	HIS	-	expression tag	UNP Q6VAL9
F	15	HIS	-	expression tag	UNP Q6VAL9
F	16	HIS	-	expression tag	UNP Q6VAL9
F	17	HIS	-	expression tag	UNP Q6VAL9
F	18	HIS	-	expression tag	UNP Q6VAL9
F	19	HIS	-	expression tag	UNP Q6VAL9
F	20	ASP	-	expression tag	UNP Q6VAL9
F	21	TYR	-	expression tag	UNP Q6VAL9
F	22	ASP	-	expression tag	UNP Q6VAL9
F	23	ILE	-	expression tag	UNP Q6VAL9
F	24	PRO	-	expression tag	UNP Q6VAL9
F	25	THR	-	expression tag	UNP Q6VAL9
F	26	THR	-	expression tag	UNP Q6VAL9
F	27	GLU	-	expression tag	UNP Q6VAL9
F	28	ASN	-	expression tag	UNP Q6VAL9
F	29	LEU	-	expression tag	UNP Q6VAL9
F	30	TYR	-	expression tag	UNP Q6VAL9
F	31	PHE	-	expression tag	UNP Q6VAL9
F	32	GLN	-	expression tag	UNP Q6VAL9
F	33	GLY	-	expression tag	UNP Q6VAL9
F	34	ALA	-	expression tag	UNP Q6VAL9
F	35	MET	-	expression tag	UNP Q6VAL9
F	36	GLY	-	expression tag	UNP Q6VAL9
F	37	SER	-	expression tag	UNP Q6VAL9
F	38	GLY	-	expression tag	UNP Q6VAL9
F	39	ILE	-	expression tag	UNP Q6VAL9
F	40	GLN	-	expression tag	UNP Q6VAL9
H	14	HIS	-	expression tag	UNP Q6VAL9
H	15	HIS	-	expression tag	UNP Q6VAL9
H	16	HIS	-	expression tag	UNP Q6VAL9
H	17	HIS	-	expression tag	UNP Q6VAL9
H	18	HIS	-	expression tag	UNP Q6VAL9
H	19	HIS	-	expression tag	UNP Q6VAL9
H	20	ASP	-	expression tag	UNP Q6VAL9
H	21	TYR	-	expression tag	UNP Q6VAL9
H	22	ASP	-	expression tag	UNP Q6VAL9
H	23	ILE	-	expression tag	UNP Q6VAL9
H	24	PRO	-	expression tag	UNP Q6VAL9

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Chain	Residue	Modelled	Actual	Comment	Reference
H	25	THR	-	expression tag	UNP Q6VAL9
H	26	THR	-	expression tag	UNP Q6VAL9
H	27	GLU	-	expression tag	UNP Q6VAL9
H	28	ASN	-	expression tag	UNP Q6VAL9
H	29	LEU	-	expression tag	UNP Q6VAL9
H	30	TYR	-	expression tag	UNP Q6VAL9
H	31	PHE	-	expression tag	UNP Q6VAL9
H	32	GLN	-	expression tag	UNP Q6VAL9
H	33	GLY	-	expression tag	UNP Q6VAL9
H	34	ALA	-	expression tag	UNP Q6VAL9
H	35	MET	-	expression tag	UNP Q6VAL9
H	36	GLY	-	expression tag	UNP Q6VAL9
H	37	SER	-	expression tag	UNP Q6VAL9
H	38	GLY	-	expression tag	UNP Q6VAL9
H	39	ILE	-	expression tag	UNP Q6VAL9
H	40	GLN	-	expression tag	UNP Q6VAL9

- Molecule 3 is a protein called C-type cytochrome c552.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	105	Total	C	N	O	S	0	0	0
			788	508	132	145	3			
3	J	102	Total	C	N	O	S	0	0	0
			769	498	129	139	3			
3	K	103	Total	C	N	O	S	0	0	0
			775	501	130	141	3			
3	L	102	Total	C	N	O	S	0	1	0
			775	502	129	141	3			

There are 40 discrepancies between the modelled and reference sequences:

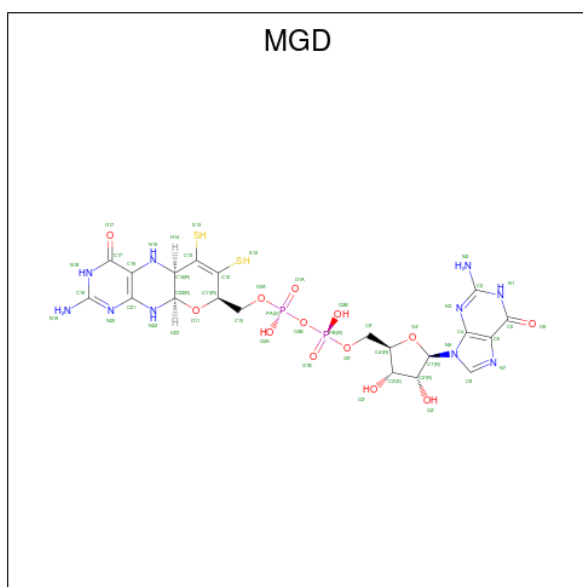
Chain	Residue	Modelled	Actual	Comment	Reference
I	19	MET	-	initiating methionine	UNP Q2TV05
I	20	ASP	-	expression tag	UNP Q2TV05
I	128	LEU	-	expression tag	UNP Q2TV05
I	129	GLU	-	expression tag	UNP Q2TV05
I	130	HIS	-	expression tag	UNP Q2TV05
I	131	HIS	-	expression tag	UNP Q2TV05
I	132	HIS	-	expression tag	UNP Q2TV05
I	133	HIS	-	expression tag	UNP Q2TV05
I	134	HIS	-	expression tag	UNP Q2TV05
I	135	HIS	-	expression tag	UNP Q2TV05

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Chain	Residue	Modelled	Actual	Comment	Reference
J	19	MET	-	initiating methionine	UNP Q2TV05
J	20	ASP	-	expression tag	UNP Q2TV05
J	128	LEU	-	expression tag	UNP Q2TV05
J	129	GLU	-	expression tag	UNP Q2TV05
J	130	HIS	-	expression tag	UNP Q2TV05
J	131	HIS	-	expression tag	UNP Q2TV05
J	132	HIS	-	expression tag	UNP Q2TV05
J	133	HIS	-	expression tag	UNP Q2TV05
J	134	HIS	-	expression tag	UNP Q2TV05
J	135	HIS	-	expression tag	UNP Q2TV05
K	19	MET	-	initiating methionine	UNP Q2TV05
K	20	ASP	-	expression tag	UNP Q2TV05
K	128	LEU	-	expression tag	UNP Q2TV05
K	129	GLU	-	expression tag	UNP Q2TV05
K	130	HIS	-	expression tag	UNP Q2TV05
K	131	HIS	-	expression tag	UNP Q2TV05
K	132	HIS	-	expression tag	UNP Q2TV05
K	133	HIS	-	expression tag	UNP Q2TV05
K	134	HIS	-	expression tag	UNP Q2TV05
K	135	HIS	-	expression tag	UNP Q2TV05
L	19	MET	-	initiating methionine	UNP Q2TV05
L	20	ASP	-	expression tag	UNP Q2TV05
L	128	LEU	-	expression tag	UNP Q2TV05
L	129	GLU	-	expression tag	UNP Q2TV05
L	130	HIS	-	expression tag	UNP Q2TV05
L	131	HIS	-	expression tag	UNP Q2TV05
L	132	HIS	-	expression tag	UNP Q2TV05
L	133	HIS	-	expression tag	UNP Q2TV05
L	134	HIS	-	expression tag	UNP Q2TV05
L	135	HIS	-	expression tag	UNP Q2TV05

- Molecule 4 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).

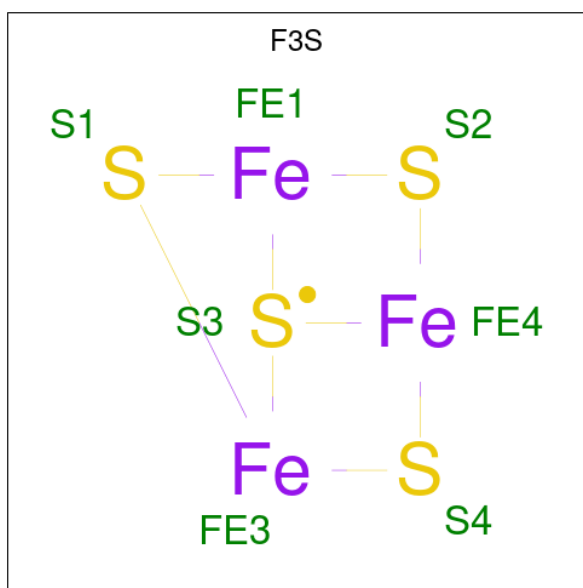


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	A	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	A	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	C	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	C	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	E	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	E	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	G	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	G	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0

- Molecule 5 is MOLYBDENUM(IV) ION (CCD ID: 4MO) (formula: Mo).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mo	0	0
			1	1		
5	C	1	Total	Mo	0	0
			1	1		
5	E	1	Total	Mo	0	0
			1	1		
5	G	1	Total	Mo	0	0
			1	1		

- Molecule 6 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).

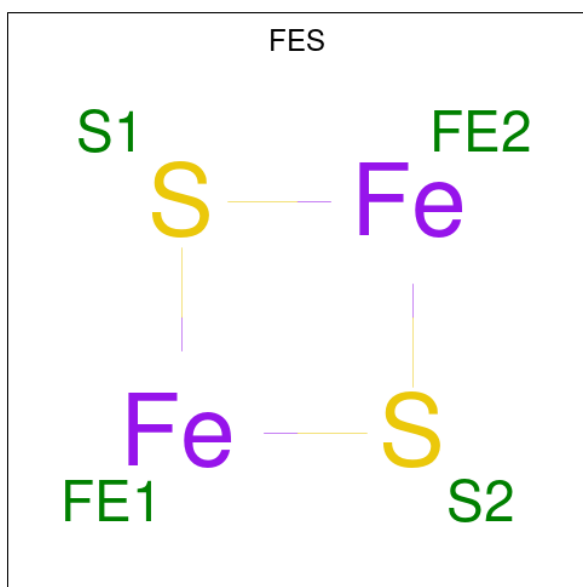


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Fe	S	0	0
			7	3	4		
6	C	1	Total	Fe	S	0	0
			7	3	4		
6	E	1	Total	Fe	S	0	0
			7	3	4		
6	G	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 7 is OXYGEN ATOM (CCD ID: O) (formula: O).

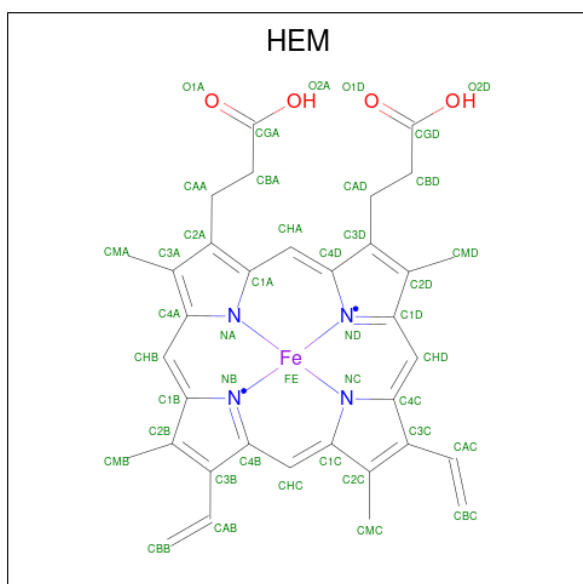
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O	0	0
			1	1		
7	C	1	Total	O	0	0
			1	1		
7	E	1	Total	O	0	0
			1	1		
7	G	1	Total	O	0	0
			1	1		

- Molecule 8 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



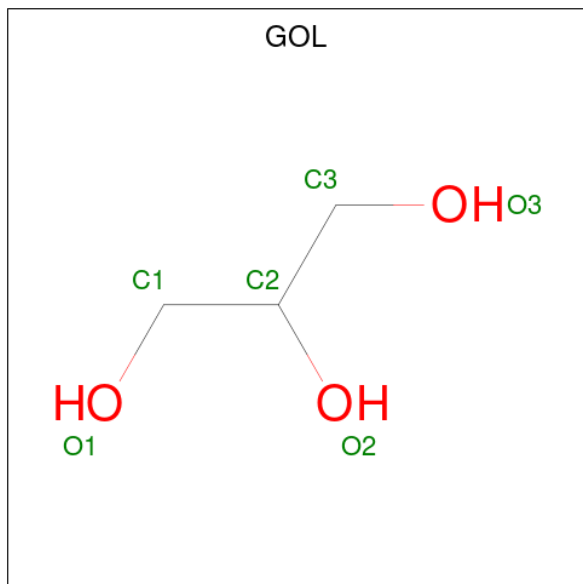
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			4	2	2		
8	D	1	Total	Fe	S	0	0
			4	2	2		
8	F	1	Total	Fe	S	0	0
			4	2	2		
8	H	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



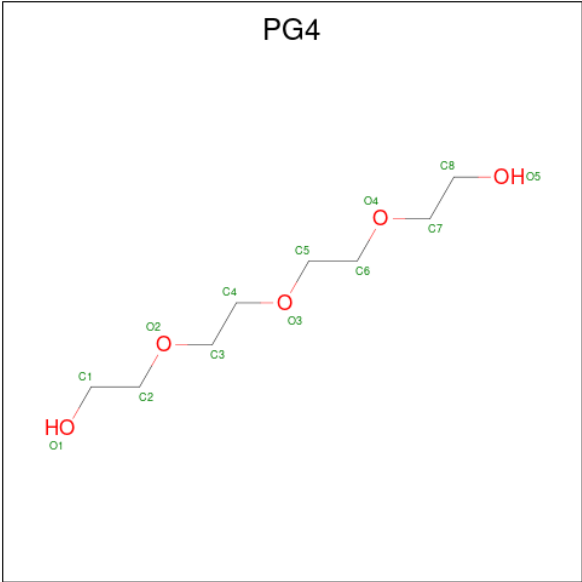
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	I	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	L	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



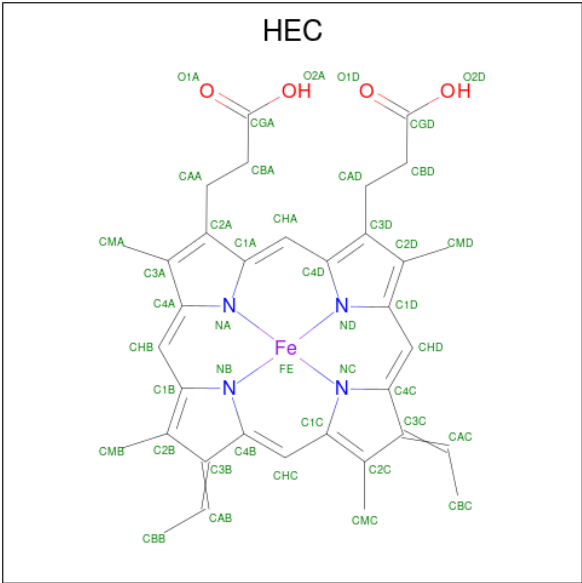
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	E	1	Total	C	O	0	0
			13	8	5		
11	G	1	Total	C	O	0	0
			13	8	5		

- Molecule 12 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	K	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

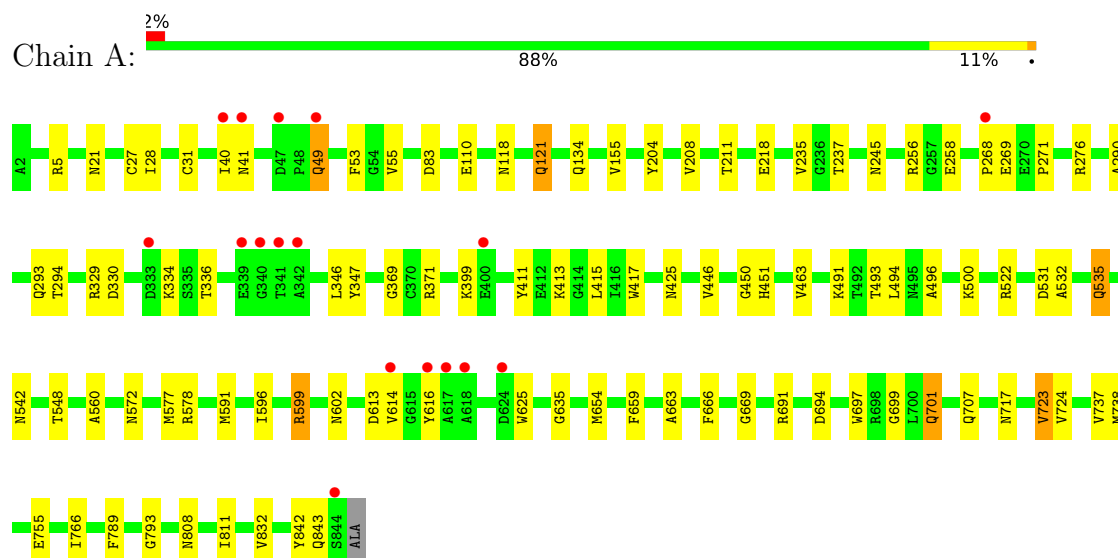
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	341	Total 341	O 341	0	0
13	B	21	Total 21	O 21	0	0
13	I	8	Total 8	O 8	0	0
13	C	281	Total 281	O 281	0	0
13	D	24	Total 24	O 24	0	0
13	J	13	Total 13	O 13	0	0
13	E	481	Total 481	O 481	0	0
13	F	73	Total 73	O 73	0	0
13	K	19	Total 19	O 19	0	0
13	G	420	Total 420	O 420	0	0
13	H	54	Total 54	O 54	0	0
13	L	14	Total 14	O 14	0	0

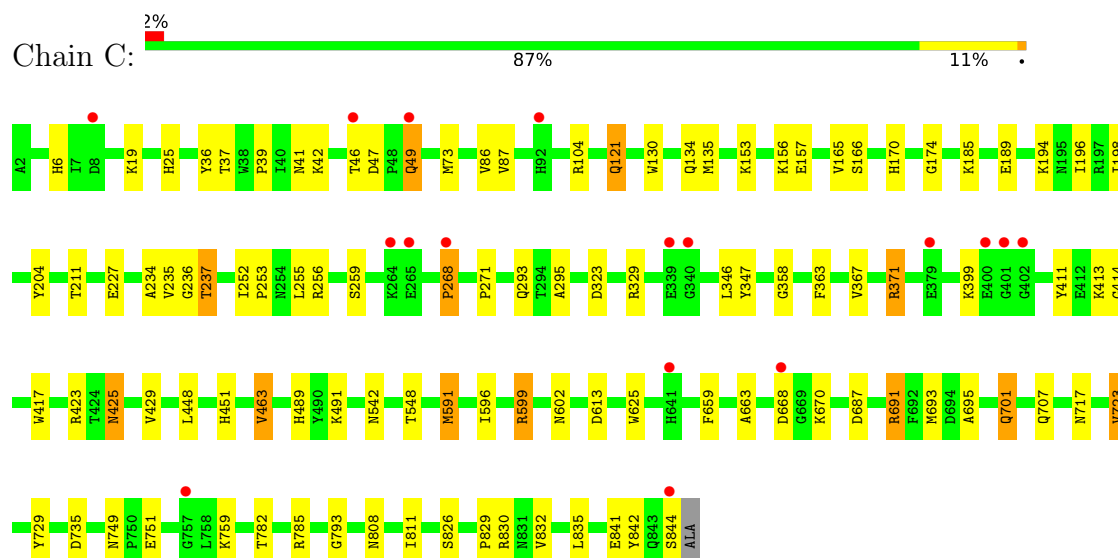
3 Residue-property plots [i](#)

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.

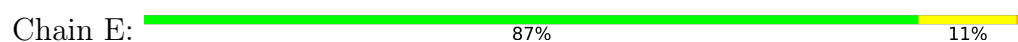
• Molecule 1: AroA

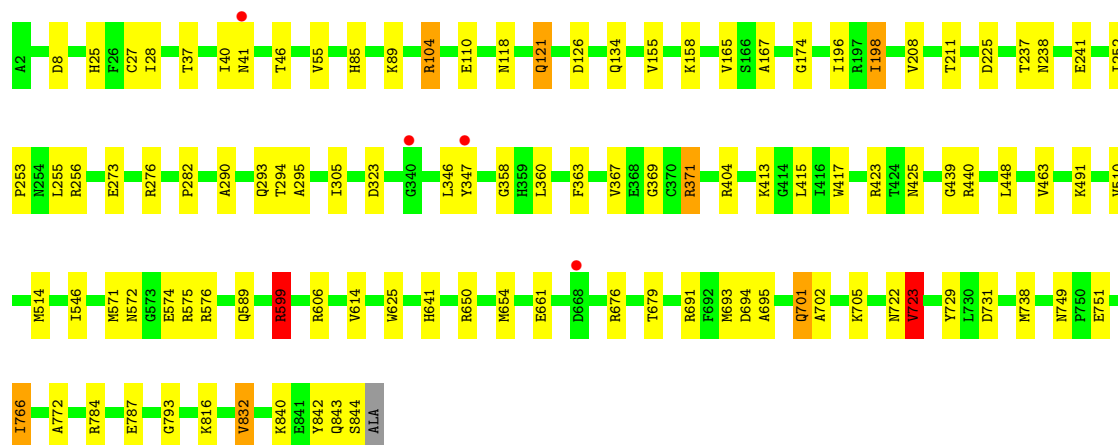


• Molecule 1: AroA



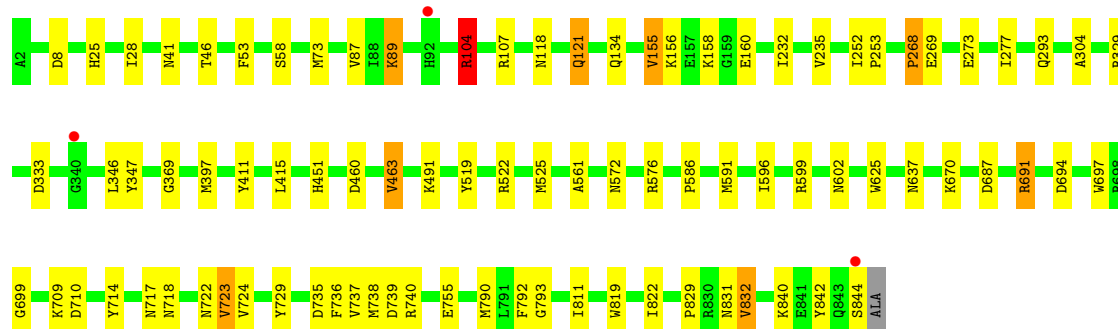
• Molecule 1: AroA





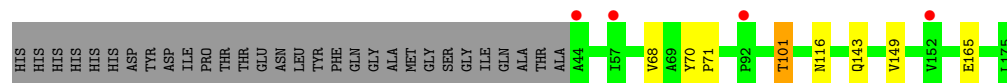
• Molecule 1: AroA

Chain G: 89% 9% .



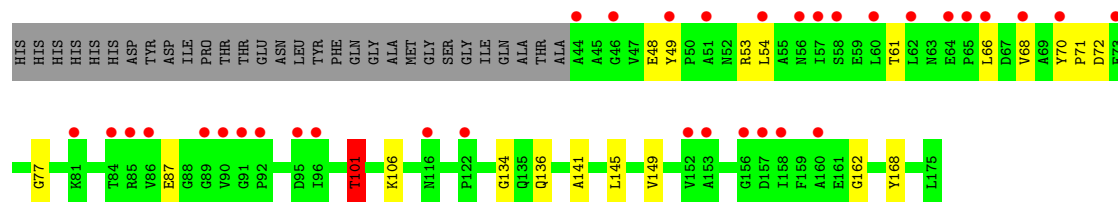
• Molecule 2: AroB

Chain B: 2% 77% 19%



• Molecule 2: AroB

Chain D: 21% 69% 12% 19%



• Molecule 2: AroB

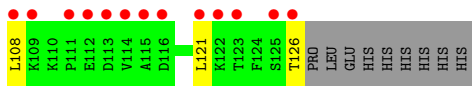
Chain F: 71% 9% 19%



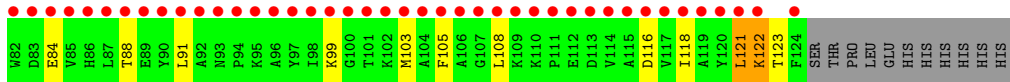
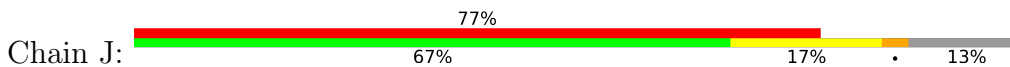
- Molecule 2: AroB



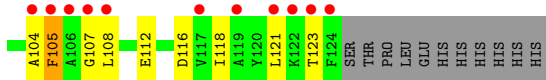
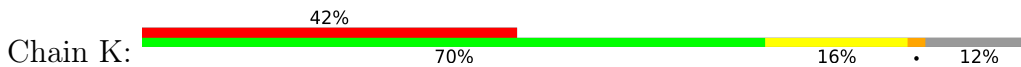
- Molecule 3: C-type cytochrome c552



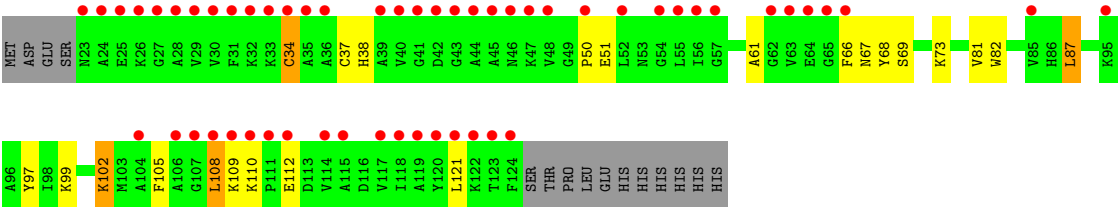
- Molecule 3: C-type cytochrome c552



- Molecule 3: C-type cytochrome c552



- Molecule 3: C-type cytochrome c552



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	129.40Å 126.56Å 148.02Å 90.00° 107.81° 90.00°	Depositor
Resolution (Å)	49.23 – 2.25 49.23 – 2.25	Depositor EDS
% Data completeness (in resolution range)	92.2 (49.23-2.25) 92.2 (49.23-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.55 (at 2.24Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.181 , 0.230 0.189 , 0.234	Depositor DCC
R_{free} test set	10062 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	3.0	Xtrriage
Anisotropy	0.533	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 30.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	35834	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.14 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.3893e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MGD, HEC, GOL, PG4, 4MO, FES, HEM, F3S, O

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	1.03	0/6738	1.37	1/9128 (0.0%)
1	C	1.02	0/6733	1.37	6/9122 (0.1%)
1	E	1.00	0/6806	1.37	4/9217 (0.0%)
1	G	1.01	0/6769	1.37	3/9169 (0.0%)
2	B	1.00	0/1018	1.30	1/1387 (0.1%)
2	D	1.07	0/1018	1.36	3/1387 (0.2%)
2	F	1.00	0/1018	1.33	1/1387 (0.1%)
2	H	0.99	0/1013	1.30	1/1380 (0.1%)
3	I	1.08	0/806	1.54	1/1088 (0.1%)
3	J	1.09	0/787	1.55	2/1062 (0.2%)
3	K	1.07	0/793	1.53	1/1070 (0.1%)
3	L	1.14	0/796	1.56	0/1074
All	All	1.02	0/34295	1.38	24/46471 (0.1%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	101	THR	CB-CA-C	7.18	122.66	111.02
3	K	107	GLY	CA-C-O	-6.15	116.91	122.57
3	J	34	CYS	CA-C-N	5.94	129.05	120.38
3	J	34	CYS	C-N-CA	5.94	129.05	120.38
1	C	723	VAL	CB-CA-C	-5.88	104.11	112.22
2	D	72	ASP	CA-C-N	5.74	128.25	120.38
2	D	72	ASP	C-N-CA	5.74	128.25	120.38
2	H	165	GLU	CB-CG-CD	5.72	122.32	112.60
1	G	104	ARG	CG-CD-NE	-5.66	99.54	112.00
1	E	198	ILE	N-CA-CB	-5.57	106.00	112.34
1	C	425	ASN	CA-C-N	5.50	126.05	119.94
1	C	425	ASN	C-N-CA	5.50	126.05	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	268	PRO	N-CA-C	-5.37	103.13	111.13
1	E	599	ARG	CG-CD-NE	-5.29	100.36	112.00
3	I	105	PHE	CA-CB-CG	5.28	119.08	113.80
2	D	101	THR	CB-CA-C	5.28	119.51	110.85
1	C	198	ILE	CA-C-O	-5.22	117.55	121.68
1	A	635	GLY	O-C-N	5.18	124.75	121.85
1	C	268	PRO	N-CA-C	-5.15	101.86	112.47
1	C	723	VAL	N-CA-CB	5.14	118.30	110.58
1	E	832	VAL	N-CA-CB	-5.12	106.24	112.33
2	B	101	THR	CB-CA-C	5.11	119.43	110.64
1	G	832	VAL	N-CA-CB	-5.10	106.60	112.21
1	E	723	VAL	CB-CA-C	-5.07	105.23	112.22

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	6577	0	6339	64	0
1	C	6573	0	6332	69	0
1	E	6624	0	6397	76	0
1	G	6597	0	6372	64	0
2	B	995	0	947	6	0
2	D	995	0	947	13	0
2	F	995	0	947	11	0
2	H	990	0	942	19	0
3	I	788	0	787	14	0
3	J	769	0	770	20	0
3	K	775	0	774	13	0
3	L	775	0	776	17	0
4	A	94	0	44	2	0
4	C	94	0	44	3	0
4	E	94	0	44	2	0
4	G	94	0	44	2	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
6	A	7	0	0	0	0
6	C	7	0	0	1	0
6	E	7	0	0	0	0
6	G	7	0	0	0	0
7	A	1	0	0	1	0
7	C	1	0	0	1	0
7	E	1	0	0	1	0
7	G	1	0	0	0	0
8	B	4	0	0	0	0
8	D	4	0	0	1	0
8	F	4	0	0	0	0
8	H	4	0	0	0	0
9	I	43	0	30	9	0
9	J	43	0	30	10	0
9	L	43	0	30	10	0
10	E	6	0	8	1	0
11	E	13	0	17	0	0
11	G	13	0	17	20	0
12	K	43	0	32	5	0
13	A	341	0	0	9	0
13	B	21	0	0	1	0
13	C	281	0	0	8	0
13	D	24	0	0	3	0
13	E	481	0	0	23	0
13	F	73	0	0	5	0
13	G	420	0	0	16	0
13	H	54	0	0	4	0
13	I	8	0	0	0	0
13	J	13	0	0	4	0
13	K	19	0	0	2	0
13	L	14	0	0	0	0
All	All	35834	0	32670	384	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 6.

All (384) 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)
3:I:34:CYS:SG	9:I:200:HEM:CAB	2.25	1.25
3:K:37:CYS:SG	12:K:200:HEC:CAC	2.28	1.22
3:L:34:CYS:SG	9:L:200:HEM:CAB	2.37	1.12
3:J:34:CYS:SG	9:J:200:HEM:CAB	2.41	1.09
2:D:87:GLU:O	13:D:301:HOH:O	1.72	1.07
3:J:34:CYS:SG	9:J:200:HEM:CBB	2.44	1.05
3:I:37:CYS:SG	9:I:200:HEM:CAC	2.47	1.03
3:I:34:CYS:SG	9:I:200:HEM:CBB	2.47	1.02
3:L:37:CYS:SG	9:L:200:HEM:CAC	2.50	1.00
3:K:37:CYS:SG	12:K:200:HEC:CBC	2.52	0.97
2:F:44:ALA:N	13:F:301:HOH:O	1.97	0.97
1:E:574:GLU:OE1	1:E:576:ARG:NH1	1.98	0.96
3:K:37:CYS:SG	12:K:200:HEC:HBC3	2.08	0.93
1:G:107:ARG:HD3	13:G:2344:HOH:O	1.69	0.93
1:C:104:ARG:NH1	6:C:2004:F3S:S2	2.42	0.92
3:L:34:CYS:SG	9:L:200:HEM:CBB	2.61	0.88
7:E:2005:O:O	13:E:2102:HOH:O	1.90	0.88
1:E:41:ASN:N	13:E:2101:HOH:O	1.79	0.85
2:H:45:ALA:N	13:H:301:HOH:O	2.09	0.83
2:F:85:ARG:NH1	3:L:97:TYR:O	2.14	0.81
1:G:710:ASP:N	13:G:2101:HOH:O	2.12	0.80
11:G:2006:PG4:H71	2:H:144:ASN:HD21	1.48	0.79
1:C:830:ARG:NH1	13:C:2103:HOH:O	2.14	0.79
1:E:641[B]:HIS:ND1	13:E:2106:HOH:O	2.15	0.79
3:L:37:CYS:HG	9:L:200:HEM:CAC	1.95	0.79
1:G:740:ARG:HB2	11:G:2006:PG4:H51	1.62	0.79
1:C:130:TRP:HE3	1:C:135:MET:HE2	1.48	0.78
1:G:121[A]:GLN:HA	1:G:121[A]:GLN:HE21	1.49	0.76
1:E:294[A]:THR:HG22	13:E:2350:HOH:O	1.85	0.75
3:K:37:CYS:SG	12:K:200:HEC:C3C	2.76	0.74
1:E:676[B]:ARG:HG3	1:E:676[B]:ARG:HH11	1.51	0.74
1:E:787:GLU:OE1	13:E:2103:HOH:O	2.04	0.74
3:J:37:CYS:SG	9:J:200:HEM:CAC	2.76	0.74
3:I:37:CYS:SG	9:I:200:HEM:CBC	2.75	0.74
1:G:709:LYS:O	13:G:2102:HOH:O	2.06	0.73
1:C:130:TRP:HB2	1:C:135:MET:HE1	1.72	0.72
1:A:737:VAL:HG12	1:A:738:MET:HE2	1.70	0.72
1:E:40:ILE:HA	13:E:2101:HOH:O	1.89	0.72
1:C:693:MET:HE2	1:C:695:ALA:HB2	1.73	0.71
1:E:118:ASN:ND2	13:E:2104:HOH:O	2.07	0.71
1:E:40:ILE:O	13:E:2105:HOH:O	2.08	0.69
7:C:2005:O:O	13:C:2101:HOH:O	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:GLN:HE21	1:C:844:SER:HB2	1.58	0.69
9:L:200:HEM:HMB1	9:L:200:HEM:HBB2	1.74	0.69
1:C:423:ARG:HA	1:C:693:MET:HE1	1.73	0.68
1:A:40:ILE:HA	13:A:2101:HOH:O	1.94	0.68
1:C:121:GLN:HE21	1:C:121:GLN:HA	1.58	0.68
1:A:49:GLN:H	1:A:49:GLN:HE21	1.42	0.67
13:E:2104:HOH:O	1:G:735:ASP:OD2	2.13	0.67
1:C:735:ASP:OD2	13:C:2102:HOH:O	2.13	0.66
1:E:256:ARG:HD3	3:K:47:LYS:HA	1.75	0.66
2:F:151:ARG:HD3	2:F:161:GLU:OE2	1.95	0.66
1:G:118:ASN:HD22	1:G:121[B]:GLN:NE2	1.92	0.66
1:A:41:ASN:N	13:A:2101:HOH:O	1.87	0.65
1:C:358:GLY:HA3	1:C:693:MET:HE3	1.78	0.65
1:C:599:ARG:NH1	1:C:602:ASN:OD1	2.29	0.65
1:E:784:ARG:N	13:E:2112:HOH:O	2.28	0.65
1:E:723:VAL:HG13	13:F:351:HOH:O	1.97	0.65
1:C:451:HIS:HE1	13:C:2164:HOH:O	1.81	0.64
1:G:121[A]:GLN:HA	1:G:121[A]:GLN:NE2	2.13	0.63
3:L:37:CYS:SG	9:L:200:HEM:CBC	2.86	0.63
1:A:118:ASN:ND2	13:C:2102:HOH:O	2.21	0.63
1:A:697:TRP:CZ2	1:A:699:GLY:HA2	2.32	0.63
1:E:40:ILE:CA	13:E:2101:HOH:O	2.46	0.63
1:A:369:GLY:HA3	1:A:694:ASP:OD1	1.98	0.63
3:I:34:CYS:SG	9:I:200:HEM:HAB	2.36	0.63
1:C:130:TRP:HB2	1:C:135:MET:CE	2.29	0.62
11:G:2006:PG4:H21	2:H:139:GLY:O	1.99	0.62
1:C:204:TYR:HB3	1:C:463:VAL:HG11	1.82	0.62
3:J:58:ARG:NE	13:J:302:HOH:O	2.32	0.62
1:G:460:ASP:O	1:G:463:VAL:HB	1.99	0.62
1:G:740:ARG:HD3	11:G:2006:PG4:H52	1.80	0.62
2:F:57:ILE:HD12	2:F:158:ILE:HD11	1.82	0.62
1:E:323:ASP:OD2	1:E:371:ARG:NH2	2.33	0.61
1:E:599:ARG:NH2	1:E:625:TRP:O	2.31	0.61
13:F:359:HOH:O	3:K:104:ALA:HB1	1.99	0.61
2:D:70:TYR:CD1	2:D:71:PRO:HA	2.36	0.61
1:C:413:LYS:HD2	1:C:417:TRP:NE1	2.16	0.61
3:K:23:ASN:HD22	3:K:26:LYS:HG2	1.65	0.61
11:G:2006:PG4:C7	2:H:144:ASN:HD21	2.12	0.61
2:B:70:TYR:CD1	2:B:71:PRO:HA	2.36	0.60
1:E:8:ASP:OD2	13:E:2107:HOH:O	2.16	0.60
1:E:121[A]:GLN:HE21	1:E:121[A]:GLN:HA	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:840:LYS:HE3	13:E:2492:HOH:O	2.02	0.60
1:E:89:LYS:CB	13:E:2553:HOH:O	2.49	0.59
1:C:829:PRO:O	1:C:832[B]:VAL:HG22	2.02	0.59
3:L:37:CYS:SG	9:L:200:HEM:C3C	2.95	0.59
2:D:134:GLY:HA3	13:D:302:HOH:O	2.02	0.59
3:I:34:CYS:SG	9:I:200:HEM:C3B	2.95	0.59
1:E:252:ILE:HD12	1:E:294[A]:THR:HG21	1.84	0.58
1:E:843:GLN:HG3	2:F:116:ASN:HD21	1.68	0.58
1:C:130:TRP:CE3	1:C:135:MET:HE2	2.35	0.58
1:G:736:PHE:CE1	11:G:2006:PG4:H62	2.39	0.58
1:A:723[B]:VAL:HG23	1:A:724:VAL:HG23	1.85	0.58
3:I:37:CYS:SG	9:I:200:HEM:C3C	2.97	0.58
1:G:736:PHE:O	11:G:2006:PG4:H72	2.04	0.58
2:D:145:LEU:O	13:D:302:HOH:O	2.17	0.57
3:L:34:CYS:SG	9:L:200:HEM:C3B	2.98	0.57
1:E:225:ASP:OD2	1:E:676[B]:ARG:NE	2.37	0.57
1:E:731:ASP:C	1:E:738:MET:HE3	2.30	0.57
1:G:697:TRP:CZ2	1:G:699:GLY:HA2	2.39	0.57
1:A:413:LYS:HD2	1:A:417:TRP:NE1	2.20	0.57
2:B:149:VAL:HG21	1:C:41:ASN:HD22	1.70	0.57
1:C:156:LYS:NZ	1:C:613:ASP:OD2	2.39	0.56
1:G:46[A]:THR:HG23	13:G:2204:HOH:O	2.04	0.56
1:E:423:ARG:HA	1:E:693[A]:MET:HE1	1.88	0.56
2:H:85:ARG:NE	13:H:302:HOH:O	2.38	0.56
3:J:84:GLU:OE2	3:J:122:LYS:NZ	2.36	0.56
1:C:153:LYS:NZ	1:C:157:GLU:OE2	2.38	0.55
1:C:293:GLN:NE2	1:C:844:SER:HB2	2.20	0.55
1:G:451:HIS:HD2	13:G:2103:HOH:O	1.89	0.55
3:I:61:ALA:HA	3:I:68:TYR:CE2	2.42	0.55
1:A:451:HIS:HE1	13:A:2180:HOH:O	1.89	0.55
1:A:843:GLN:HE21	2:B:116:ASN:HD21	1.52	0.55
1:E:208:VAL:HB	1:E:211:THR:HG22	1.88	0.55
1:E:46:THR:HG23	13:E:2124:HOH:O	2.07	0.55
3:L:37:CYS:HG	9:L:200:HEM:CBC	2.20	0.54
1:A:83:ASP:OD2	1:C:6:HIS:CE1	2.60	0.54
1:C:599:ARG:NH2	1:C:625:TRP:O	2.40	0.54
3:I:34:CYS:HG	9:I:200:HEM:CAB	2.18	0.54
1:G:118:ASN:HD22	1:G:121[B]:GLN:HE21	1.53	0.54
1:A:531:ASP:O	1:A:535:GLN:HG2	2.07	0.54
1:E:589:GLN:HG2	13:E:2160:HOH:O	2.08	0.54
3:K:87:LEU:HD23	3:K:118:ILE:HG12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:268:PRO:HA	13:G:2104:HOH:O	2.08	0.54
2:F:149:VAL:HG21	1:G:41:ASN:HD22	1.73	0.54
2:D:54:LEU:HD13	2:D:68:VAL:HG11	1.90	0.53
3:J:37:CYS:SG	9:J:200:HEM:C3C	3.00	0.53
1:E:290:ALA:O	1:E:294[A]:THR:HG23	2.08	0.53
1:G:723[B]:VAL:HG23	1:G:724:VAL:HG23	1.89	0.53
1:A:451:HIS:HD2	13:A:2103:HOH:O	1.91	0.53
1:E:104:ARG:NH2	1:E:722:ASN:OD1	2.41	0.53
1:A:204:TYR:HB3	1:A:463:VAL:HG11	1.91	0.53
1:C:751:GLU:OE2	1:C:785:ARG:HD2	2.09	0.53
1:E:174:GLY:HA2	4:E:2001:MGD:C6	2.38	0.53
1:C:717:ASN:OD1	4:C:2002:MGD:H8	2.09	0.52
1:G:121[A]:GLN:HE21	1:G:121[A]:GLN:CA	2.13	0.52
1:G:736:PHE:O	11:G:2006:PG4:C7	2.58	0.52
1:G:739:ASP:HB3	11:G:2006:PG4:H72	1.92	0.52
11:G:2006:PG4:C3	2:H:136:GLN:HE21	2.21	0.52
1:E:676[B]:ARG:HG3	1:E:676[B]:ARG:NH1	2.21	0.52
1:A:737:VAL:HG12	1:A:738:MET:CE	2.40	0.52
1:C:135:MET:HE3	13:C:2146:HOH:O	2.10	0.52
3:J:58:ARG:CD	13:J:302:HOH:O	2.58	0.52
1:G:840:LYS:CE	13:G:2413:HOH:O	2.58	0.52
1:A:599:ARG:NH1	1:A:602:ASN:OD1	2.38	0.52
3:L:50:PRO:HD3	3:L:66:PHE:CZ	2.45	0.52
1:A:330:ASP:OD1	1:A:334:LYS:HD3	2.10	0.51
3:I:84:GLU:N	3:I:84:GLU:OE1	2.43	0.51
1:C:255:LEU:HB3	1:C:295:ALA:HB2	1.92	0.51
11:G:2006:PG4:H62	2:H:144:ASN:OD1	2.10	0.51
1:G:397:MET:HE2	13:G:2459:HOH:O	2.10	0.51
11:G:2006:PG4:H32	2:H:136:GLN:HE21	1.75	0.51
1:E:693[A]:MET:HE2	1:E:695:ALA:HB2	1.91	0.51
1:G:155:VAL:HG22	1:G:160:GLU:HA	1.93	0.51
1:A:211:THR:H	1:A:425:ASN:ND2	2.09	0.51
1:C:236:GLY:HA3	1:C:414:GLY:HA3	1.93	0.51
1:G:293:GLN:NE2	1:G:844:SER:OG	2.44	0.51
1:G:737:VAL:HG12	1:G:738:MET:HE2	1.91	0.50
3:L:69:SER:HB3	3:L:102:LYS:HG2	1.92	0.50
1:C:271:PRO:HG2	1:C:399:LYS:HB3	1.93	0.50
2:D:136:GLN:OE1	2:D:141:ALA:HB3	2.11	0.50
1:A:542:ASN:ND2	1:A:548:THR:OG1	2.44	0.50
1:E:252:ILE:N	1:E:253:PRO:HD2	2.26	0.50
1:A:293:GLN:HG3	13:A:2318:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:GLY:HA2	4:C:2001:MGD:C6	2.42	0.50
1:G:491:LYS:O	1:G:793:GLY:HA2	2.12	0.50
1:E:293:GLN:HG2	1:E:842:TYR:CE2	2.47	0.50
1:G:599:ARG:NH2	1:G:625:TRP:O	2.41	0.50
1:C:687:ASP:OD2	1:C:691:ARG:NH2	2.45	0.49
1:A:21:ASN:HB2	13:A:2102:HOH:O	2.11	0.49
1:A:717:ASN:OD1	4:A:2002:MGD:H8	2.13	0.49
1:A:41:ASN:HD22	2:D:149:VAL:HG21	1.78	0.49
3:I:34:CYS:HG	9:I:200:HEM:CBB	2.25	0.49
1:C:591:MET:CG	1:C:596:ILE:HG13	2.42	0.49
1:A:415:LEU:HD23	1:A:415:LEU:C	2.38	0.49
1:G:687:ASP:OD1	1:G:691:ARG:NH2	2.46	0.49
1:E:360:LEU:HD23	1:E:693[A]:MET:HG3	1.95	0.49
1:C:693:MET:HE2	1:C:695:ALA:CB	2.43	0.49
1:E:225:ASP:OD2	1:E:676[B]:ARG:CZ	2.61	0.49
1:E:404[A]:ARG:HD2	13:E:2344:HOH:O	2.12	0.48
1:E:701:GLN:C	1:E:701:GLN:CD	2.81	0.48
2:B:70:TYR:CG	2:B:71:PRO:HA	2.49	0.48
1:C:185:LYS:O	1:C:189:GLU:HB3	2.13	0.48
1:G:415:LEU:C	1:G:415:LEU:HD23	2.39	0.48
1:A:40:ILE:CA	13:A:2101:HOH:O	2.55	0.48
1:C:235:VAL:O	1:C:411:TYR:HA	2.13	0.48
3:J:58:ARG:HD2	13:J:302:HOH:O	2.14	0.48
1:E:211:THR:H	1:E:425:ASN:ND2	2.12	0.48
1:E:491:LYS:O	1:E:793:GLY:HA2	2.13	0.48
3:J:118:ILE:CD1	13:J:301:HOH:O	2.61	0.48
2:H:70:TYR:CD1	2:H:71:PRO:HA	2.48	0.48
3:L:61:ALA:HA	3:L:68:TYR:CZ	2.49	0.48
1:E:293:GLN:HG3	13:E:2209:HOH:O	2.13	0.48
11:G:2006:PG4:C6	2:H:144:ASN:OD1	2.62	0.47
3:L:67:ASN:O	3:L:102:LYS:NZ	2.47	0.47
1:C:234:ALA:HB1	1:C:237:THR:CG2	2.45	0.47
1:C:37:THR:HG22	1:C:86:VAL:HG23	1.96	0.47
1:C:211:THR:H	1:C:425:ASN:ND2	2.13	0.47
1:C:591:MET:HG2	1:C:596:ILE:CG1	2.44	0.47
1:E:729:TYR:CD2	4:E:2001:MGD:H2'	2.48	0.47
1:G:740:ARG:CB	11:G:2006:PG4:H51	2.40	0.47
1:C:46:THR:HG23	13:C:2110:HOH:O	2.15	0.47
1:C:47:ASP:HB3	1:C:49:GLN:OE1	2.15	0.47
1:C:782:THR:HG21	1:C:841:GLU:OE2	2.15	0.47
1:E:165:VAL:O	1:E:196:ILE:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:PRO:HB2	1:C:42:LYS:HG2	1.96	0.47
1:E:606:ARG:HG2	1:E:606:ARG:HH11	1.78	0.47
11:G:2006:PG4:O3	2:H:136:GLN:HB3	2.14	0.47
1:A:268:PRO:HA	13:A:2113:HOH:O	2.14	0.47
3:K:112:GLU:O	3:K:116:ASP:OD2	2.33	0.47
1:A:577:MET:O	1:A:578:ARG:HD3	2.15	0.47
1:E:358:GLY:HA3	1:E:693[A]:MET:HE3	1.95	0.47
1:A:290:ALA:O	1:A:294:THR:HG23	2.15	0.47
1:A:599:ARG:NH2	1:A:625:TRP:O	2.38	0.47
1:A:723[B]:VAL:HG12	13:B:308:HOH:O	2.15	0.47
1:E:571:MET:HA	1:E:576:ARG:O	2.15	0.47
1:G:73:MET:O	1:G:87:VAL:HA	2.15	0.47
1:A:701:GLN:C	1:A:701:GLN:CD	2.83	0.46
1:G:740:ARG:HG2	11:G:2006:PG4:H42	1.97	0.46
1:E:37:THR:HA	1:E:85:HIS:O	2.15	0.46
1:E:702:ALA:HB3	1:E:705:LYS:HG3	1.97	0.46
1:G:104:ARG:NH2	1:G:722:ASN:OD1	2.48	0.46
1:G:451:HIS:HE1	13:G:2176:HOH:O	1.99	0.46
1:A:208:VAL:HB	1:A:211:THR:HG22	1.98	0.46
1:E:323:ASP:CG	1:E:371:ARG:HH22	2.24	0.46
1:G:687:ASP:CG	1:G:691:ARG:HH22	2.24	0.46
1:E:369:GLY:HA3	1:E:694:ASP:OD1	2.15	0.46
1:G:28:ILE:O	1:G:572:ASN:HB2	2.16	0.46
3:L:38:HIS:ND1	3:L:50:PRO:O	2.48	0.46
3:L:82:TRP:CE3	3:L:87:LEU:CD1	2.99	0.46
1:A:701:GLN:OE1	1:A:808:ASN:HA	2.16	0.46
3:K:105:PHE:HD1	13:K:319:HOH:O	1.99	0.46
1:C:423:ARG:HA	1:C:693:MET:CE	2.43	0.46
1:E:650:ARG:O	1:E:654:MET:HG3	2.16	0.46
3:J:50:PRO:HD3	3:J:66:PHE:CE2	2.51	0.45
1:E:89:LYS:HB2	13:E:2553:HOH:O	2.13	0.45
1:E:413:LYS:HD2	1:E:417:TRP:NE1	2.31	0.45
1:A:5:ARG:NE	1:A:110:GLU:OE1	2.40	0.45
1:C:425:ASN:O	1:C:429:VAL:HG23	2.16	0.45
1:C:491:LYS:O	1:C:793:GLY:HA2	2.15	0.45
11:G:2006:PG4:C8	2:H:135:GLN:HE21	2.29	0.45
2:D:49:TYR:CD1	2:D:162:GLY:HA2	2.52	0.45
2:D:77:GLY:HA2	2:D:101:THR:HB	1.99	0.45
1:C:252:ILE:N	1:C:253:PRO:HD2	2.31	0.45
3:J:37:CYS:SG	9:J:200:HEM:CBC	3.04	0.45
1:E:510:VAL:O	1:E:514:MET:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:46[A]:THR:OG1	1:G:58:SER:N	2.50	0.45
1:G:717:ASN:OD1	4:G:2002:MGD:H8	2.17	0.45
1:G:829:PRO:HB2	1:G:831:ASN:OD1	2.16	0.45
2:H:70:TYR:CG	2:H:71:PRO:HA	2.52	0.45
1:A:560:ALA:HA	1:A:591:MET:O	2.17	0.45
2:D:70:TYR:CG	2:D:71:PRO:HA	2.52	0.45
9:J:200:HEM:HMB2	9:J:200:HEM:HBB2	1.98	0.45
1:G:736:PHE:O	11:G:2006:PG4:O4	2.34	0.45
1:C:227:GLU:O	1:C:259:SER:OG	2.21	0.45
1:G:25:HIS:HD2	13:G:2156:HOH:O	2.00	0.45
1:A:256[B]:ARG:NE	1:A:258:GLU:OE2	2.50	0.45
1:C:293:GLN:HG2	1:C:842:TYR:HE1	1.81	0.45
1:C:25:HIS:HD2	13:C:2185:HOH:O	1.99	0.45
1:E:676[B]:ARG:NH1	1:E:676[B]:ARG:CG	2.79	0.45
1:A:293:GLN:HG2	1:A:842:TYR:CE2	2.52	0.45
1:G:293:GLN:HG2	1:G:842:TYR:CE2	2.52	0.44
1:A:271:PRO:HG2	1:A:399:LYS:HB3	1.98	0.44
1:G:269:GLU:N	13:G:2104:HOH:O	2.24	0.44
1:G:561:ALA:HB2	1:G:586:PRO:HB3	2.00	0.44
2:H:54:LEU:HD11	2:H:160:ALA:HB2	1.98	0.44
1:A:666:PHE:CZ	1:A:669:GLY:HA2	2.51	0.44
1:E:255:LEU:HB3	1:E:295:ALA:HB2	1.98	0.44
1:E:599:ARG:HA	1:E:599:ARG:HD3	1.58	0.44
1:A:496:ALA:O	1:A:500:LYS:HE2	2.18	0.44
7:A:2005:O:O	13:A:2103:HOH:O	2.20	0.44
1:C:19:LYS:HG3	1:C:36:TYR:CE1	2.53	0.44
1:C:73:MET:O	1:C:87:VAL:HA	2.18	0.44
1:G:599:ARG:NH1	1:G:602:ASN:OD1	2.47	0.44
2:H:85:ARG:NH2	13:H:302:HOH:O	2.51	0.44
1:E:158:LYS:HE2	13:E:2520:HOH:O	2.17	0.44
3:K:82:TRP:HB3	3:K:87:LEU:HD13	2.00	0.44
1:E:238:ASN:ND2	1:E:241:GLU:OE2	2.48	0.44
1:A:41:ASN:ND2	2:D:149:VAL:HG21	2.32	0.43
12:K:200:HEC:HMB1	12:K:200:HEC:HBB3	1.99	0.43
1:G:840:LYS:HE3	13:G:2413:HOH:O	2.18	0.43
1:C:659:PHE:CE2	1:C:663:ALA:HB2	2.53	0.43
3:J:55:LEU:HD23	3:J:121:LEU:HG	1.99	0.43
13:F:359:HOH:O	3:K:104:ALA:CB	2.64	0.43
3:K:48:VAL:HG23	13:K:312:HOH:O	2.18	0.43
1:G:8:ASP:HB3	2:H:47:VAL:HG21	2.00	0.43
1:E:572:ASN:C	1:E:574:GLU:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:ALA:HA	1:A:535:GLN:HG3	2.00	0.43
11:G:2006:PG4:H71	2:H:144:ASN:ND2	2.25	0.43
2:B:143:GLN:OE1	2:B:165:GLU:HG3	2.19	0.43
1:C:166:SER:CB	1:C:489:HIS:HE2	2.32	0.43
1:C:591:MET:HG2	1:C:596:ILE:HG13	2.00	0.43
1:E:766:ILE:O	1:E:772:ALA:HA	2.19	0.43
2:F:124:HIS:C	2:F:125:PHE:CD2	2.96	0.43
2:D:106:LYS:HB2	8:D:201:FES:S2	2.59	0.43
1:E:273[A]:GLU:HG2	13:E:2459:HOH:O	2.18	0.43
1:G:53:PHE:CE1	1:G:89:LYS:HE3	2.53	0.43
3:J:52:LEU:HD23	3:J:58:ARG:HH12	1.84	0.43
1:E:293:GLN:HG2	1:E:842:TYR:HE2	1.84	0.43
1:A:599:ARG:HD3	1:A:599:ARG:HA	1.60	0.43
9:J:200:HEM:HBB2	9:J:200:HEM:CMB	2.48	0.43
2:F:70:TYR:CD1	2:F:71:PRO:HA	2.53	0.43
1:G:737:VAL:HG12	1:G:738:MET:CE	2.48	0.43
2:H:85:ARG:CZ	13:H:302:HOH:O	2.66	0.43
3:L:105:PHE:HZ	3:L:108:LEU:HD13	1.83	0.43
1:A:268:PRO:O	1:A:269:GLU:HB2	2.19	0.42
1:G:235:VAL:O	1:G:411:TYR:HA	2.19	0.42
1:A:293:GLN:HG2	1:A:842:TYR:CD2	2.54	0.42
1:C:599:ARG:HA	1:C:599:ARG:HD3	1.71	0.42
1:G:232:ILE:O	1:G:277:ILE:HA	2.19	0.42
1:G:591:MET:HG2	1:G:596:ILE:HG12	2.00	0.42
1:G:718:ASN:HA	1:G:790:MET:O	2.19	0.42
1:A:235:VAL:O	1:A:411:TYR:HA	2.19	0.42
1:A:491:LYS:O	1:A:793:GLY:HA2	2.19	0.42
3:J:91:LEU:O	3:J:108:LEU:N	2.52	0.42
1:C:293:GLN:HG2	1:C:842:TYR:CE1	2.54	0.42
2:F:44:ALA:N	13:F:308:HOH:O	2.52	0.42
1:G:714:TYR:CD1	1:G:822:ILE:HD12	2.55	0.42
9:L:200:HEM:HMC2	9:L:200:HEM:HBC2	2.01	0.42
1:C:363:PHE:O	1:C:367:VAL:HG23	2.20	0.42
1:C:701:GLN:OE1	1:C:808:ASN:HA	2.20	0.42
1:G:252:ILE:N	1:G:253:PRO:HD2	2.34	0.42
1:G:709:LYS:HA	1:G:819:TRP:CG	2.55	0.42
1:A:121:GLN:HE21	1:A:121:GLN:HA	1.84	0.42
1:A:659:PHE:CE2	1:A:663:ALA:HB2	2.53	0.42
3:J:72:PHE:HE2	9:J:200:HEM:O2A	2.03	0.42
2:D:168:TYR:CD1	2:D:168:TYR:C	2.98	0.42
1:E:110:GLU:CD	10:E:2006:GOL:H11	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:440:ARG:C	1:E:676[B]:ARG:HH12	2.28	0.42
2:H:102:ILE:HG22	2:H:107:GLY:HA2	2.01	0.42
3:J:55:LEU:HD23	3:J:121:LEU:CD2	2.50	0.42
1:G:369:GLY:HA3	1:G:694:ASP:OD1	2.20	0.42
1:C:256:ARG:HD3	3:J:47:LYS:HA	2.01	0.41
1:C:323:ASP:OD2	1:C:371:ARG:NH2	2.53	0.41
1:E:25:HIS:HD2	13:E:2118:HOH:O	2.03	0.41
1:E:749:ASN:OD1	1:E:751:GLU:HB2	2.20	0.41
1:A:256[B]:ARG:NH2	1:A:258:GLU:OE2	2.53	0.41
2:F:54:LEU:HD13	2:F:68:VAL:HG11	2.02	0.41
3:I:50:PRO:HD3	3:I:66:PHE:CZ	2.55	0.41
1:E:575:ARG:NH1	1:E:661:GLU:O	2.48	0.41
1:A:28:ILE:O	1:A:572:ASN:HB2	2.20	0.41
1:A:717:ASN:O	1:A:789:PHE:HA	2.21	0.41
1:E:415:LEU:C	1:E:415:LEU:HD23	2.45	0.41
1:A:53:PHE:O	1:A:55:VAL:HG23	2.20	0.41
1:C:542:ASN:ND2	1:C:548:THR:OG1	2.53	0.41
3:J:103:MET:HE1	9:J:200:HEM:NB	2.35	0.41
1:E:167:ALA:O	1:E:198:ILE:HA	2.21	0.41
1:G:729:TYR:CD1	4:G:2001:MGD:H2'	2.56	0.41
1:G:740:ARG:HB2	11:G:2006:PG4:C5	2.43	0.41
1:A:31:CYS:SG	1:A:245:ASN:HB2	2.61	0.41
1:A:256[B]:ARG:HD2	3:I:47:LYS:HA	2.01	0.41
1:A:577:MET:C	1:A:578:ARG:HD3	2.46	0.41
1:C:165:VAL:O	1:C:196:ILE:HA	2.21	0.41
1:E:126:ASP:OD1	13:E:2108:HOH:O	2.22	0.41
3:L:82:TRP:CE3	3:L:87:LEU:HD13	2.56	0.41
1:A:493:THR:HG23	1:A:494:LEU:O	2.21	0.41
1:C:170:HIS:HB2	1:C:451:HIS:HB2	2.03	0.41
1:E:28:ILE:HG21	1:E:448:LEU:O	2.22	0.41
1:A:155:VAL:HG11	1:A:616:TYR:OH	2.22	0.40
3:I:89:GLU:HB3	3:I:97:TYR:CD1	2.56	0.40
1:E:282:PRO:HB3	1:E:305:ILE:O	2.21	0.40
1:E:439:GLY:O	1:E:679:THR:HG22	2.21	0.40
1:G:519:TYR:HD1	1:G:525:MET:HE3	1.86	0.40
1:A:40:ILE:O	1:A:41:ASN:HB2	2.20	0.40
1:A:413:LYS:HD2	1:A:417:TRP:CE2	2.57	0.40
2:B:143:GLN:HB3	2:B:165:GLU:HG2	2.03	0.40
1:C:729:TYR:CD1	4:C:2001:MGD:H2'	2.56	0.40
3:J:34:CYS:SG	9:J:200:HEM:C3B	3.10	0.40
1:G:576:ARG:NH2	13:G:2114:HOH:O	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:637:ASN:ND2	13:G:2135:HOH:O	2.54	0.40
1:A:218:GLU:O	1:A:446:VAL:HA	2.21	0.40
1:A:450:GLY:HA2	4:A:2002:MGD:C12	2.50	0.40
3:J:43:GLY:O	3:J:44:ALA:C	2.63	0.40
1:E:363:PHE:O	1:E:367:VAL:HG23	2.22	0.40
1:C:237:THR:HG21	1:C:448:LEU:CD1	2.52	0.40
1:C:749:ASN:OD1	1:C:751:GLU:HB2	2.21	0.40
1:E:417:TRP:HB2	1:E:816:LYS:HG2	2.04	0.40
1:A:591:MET:HG2	1:A:596:ILE:CG1	2.52	0.40
2:F:54:LEU:HD11	2:F:160:ALA:HB2	2.04	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	846/844 (100%)	793 (94%)	51 (6%)	2 (0%)	43	50
1	C	846/844 (100%)	803 (95%)	41 (5%)	2 (0%)	43	50
1	E	853/844 (101%)	813 (95%)	40 (5%)	0	100	100
1	G	850/844 (101%)	811 (95%)	37 (4%)	2 (0%)	43	50
2	B	130/162 (80%)	120 (92%)	10 (8%)	0	100	100
2	D	130/162 (80%)	120 (92%)	10 (8%)	0	100	100
2	F	130/162 (80%)	117 (90%)	13 (10%)	0	100	100
2	H	129/162 (80%)	122 (95%)	7 (5%)	0	100	100
3	I	103/117 (88%)	97 (94%)	5 (5%)	1 (1%)	12	10
3	J	100/117 (86%)	84 (84%)	15 (15%)	1 (1%)	12	10
3	K	101/117 (86%)	91 (90%)	9 (9%)	1 (1%)	12	10
3	L	101/117 (86%)	95 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4319/4492 (96%)	4066 (94%)	244 (6%)	9 (0%)	43 50

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	105	PHE
3	J	105	PHE
3	K	105	PHE
1	A	613	ASP
1	C	668	ASP
1	A	811	ILE
1	G	304	ALA
1	G	811	ILE
1	C	811	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	682/677 (101%)	658 (96%)	24 (4%)	32 39
1	C	682/677 (101%)	663 (97%)	19 (3%)	38 48
1	E	689/677 (102%)	667 (97%)	22 (3%)	34 43
1	G	686/677 (101%)	663 (97%)	23 (3%)	32 40
2	B	105/129 (81%)	103 (98%)	2 (2%)	50 61
2	D	105/129 (81%)	100 (95%)	5 (5%)	23 25
2	F	105/129 (81%)	101 (96%)	4 (4%)	29 36
2	H	105/129 (81%)	103 (98%)	2 (2%)	50 61
3	I	77/89 (86%)	68 (88%)	9 (12%)	5 3
3	J	74/89 (83%)	66 (89%)	8 (11%)	6 4
3	K	75/89 (84%)	66 (88%)	9 (12%)	5 3
3	L	75/89 (84%)	63 (84%)	12 (16%)	2 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3460/3580 (97%)	3321 (96%)	139 (4%)	28	34

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	CYS
1	A	49	GLN
1	A	121	GLN
1	A	134	GLN
1	A	237	THR
1	A	276	ARG
1	A	329	ARG
1	A	336	THR
1	A	346	LEU
1	A	347	TYR
1	A	371	ARG
1	A	522	ARG
1	A	535	GLN
1	A	599	ARG
1	A	614	VAL
1	A	654	MET
1	A	691	ARG
1	A	701	GLN
1	A	707	GLN
1	A	723[A]	VAL
1	A	723[B]	VAL
1	A	755	GLU
1	A	766	ILE
1	A	832	VAL
2	B	68	VAL
2	B	101	THR
3	I	26	LYS
3	I	32	LYS
3	I	51	GLU
3	I	59	LYS
3	I	77	GLU
3	I	88	THR
3	I	108	LEU
3	I	121	LEU
3	I	126	THR
1	C	49	GLN
1	C	121	GLN

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Mol	Chain	Res	Type
1	C	134	GLN
1	C	194	LYS
1	C	237	THR
1	C	329	ARG
1	C	346	LEU
1	C	347	TYR
1	C	371	ARG
1	C	463	VAL
1	C	591	MET
1	C	599	ARG
1	C	670	LYS
1	C	691	ARG
1	C	701	GLN
1	C	707	GLN
1	C	723	VAL
1	C	759	LYS
1	C	826	SER
2	D	48	GLU
2	D	53	ARG
2	D	61	THR
2	D	66	LEU
2	D	101	THR
3	J	51	GLU
3	J	58	ARG
3	J	88	THR
3	J	99	LYS
3	J	116	ASP
3	J	121	LEU
3	J	122	LYS
3	J	123	THR
1	E	27	CYS
1	E	55	VAL
1	E	104	ARG
1	E	121[A]	GLN
1	E	121[B]	GLN
1	E	134	GLN
1	E	155	VAL
1	E	237	THR
1	E	276	ARG
1	E	346	LEU
1	E	347	TYR
1	E	371	ARG

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Mol	Chain	Res	Type
1	E	463	VAL
1	E	546	ILE
1	E	599	ARG
1	E	614	VAL
1	E	691	ARG
1	E	701	GLN
1	E	723	VAL
1	E	766	ILE
1	E	832	VAL
1	E	844	SER
2	F	57	ILE
2	F	84	THR
2	F	85	ARG
2	F	101	THR
3	K	26	LYS
3	K	51	GLU
3	K	72	PHE
3	K	81	VAL
3	K	84	GLU
3	K	88	THR
3	K	108	LEU
3	K	121	LEU
3	K	123	THR
1	G	89	LYS
1	G	104	ARG
1	G	121[A]	GLN
1	G	121[B]	GLN
1	G	134	GLN
1	G	155	VAL
1	G	156	LYS
1	G	158	LYS
1	G	273	GLU
1	G	329[A]	ARG
1	G	329[B]	ARG
1	G	333	ASP
1	G	346	LEU
1	G	347	TYR
1	G	463	VAL
1	G	522	ARG
1	G	670	LYS
1	G	691	ARG
1	G	723[A]	VAL

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Mol	Chain	Res	Type
1	G	723[B]	VAL
1	G	755	GLU
1	G	792	PHE
1	G	832	VAL
2	H	68	VAL
2	H	101	THR
3	L	34	CYS
3	L	51	GLU
3	L	73	LYS
3	L	81	VAL
3	L	87	LEU
3	L	99	LYS
3	L	102	LYS
3	L	108	LEU
3	L	109	LYS
3	L	110	LYS
3	L	112	GLU
3	L	121	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	34	HIS
1	A	41	ASN
1	A	49	GLN
1	A	61	GLN
1	A	79	GLN
1	A	118	ASN
1	A	121	GLN
1	A	220	ASN
1	A	293	GLN
1	A	425	ASN
1	A	451	HIS
1	A	542	ASN
2	B	116	ASN
2	B	120	ASN
1	C	6	HIS
1	C	25	HIS
1	C	41	ASN
1	C	61	GLN
1	C	62	GLN

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Mol	Chain	Res	Type
1	C	118	ASN
1	C	121	GLN
1	C	220	ASN
1	C	425	ASN
1	C	451	HIS
1	C	472	GLN
1	C	542	ASN
1	C	637	ASN
1	C	843	GLN
1	E	6	HIS
1	E	25	HIS
1	E	34	HIS
1	E	41	ASN
1	E	49	GLN
1	E	61	GLN
1	E	118	ASN
1	E	134	GLN
1	E	195	ASN
1	E	220	ASN
1	E	299	ASN
1	E	359	HIS
1	E	425	ASN
1	E	542	ASN
1	E	708	GLN
2	F	116	ASN
3	K	23	ASN
1	G	34	HIS
1	G	41	ASN
1	G	293	GLN
1	G	359	HIS
1	G	451	HIS
1	G	542	ASN
1	G	637	ASN
2	H	116	ASN
2	H	143	GLN
3	L	23	ASN

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 31 ligands modelled in this entry, 8 are monoatomic - leaving 23 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$
10	GOL	E	2006	-	5,5,5	0.16	0	5,5,5	0.19	0
8	FES	H	201	2	0,4,4	-	-	-		
6	F3S	G	2004	1	0,9,9	-	-	-		
4	MGD	G	2001	5	47,52,52	0.55	0	58,81,81	0.99	4 (6%)
11	PG4	E	2007	-	12,12,12	0.39	0	11,11,11	0.20	0
9	HEM	I	200	3	50,50,50	1.58	6 (12%)	67,82,82	1.58	10 (14%)
4	MGD	A	2002	5	47,52,52	0.53	0	58,81,81	1.04	5 (8%)
8	FES	F	201	2	0,4,4	-	-	-		
9	HEM	L	200	3	50,50,50	1.60	5 (10%)	67,82,82	1.57	14 (20%)
6	F3S	C	2004	1	0,9,9	-	-	-		
4	MGD	G	2002	5	47,52,52	0.59	0	58,81,81	1.16	5 (8%)
4	MGD	A	2001	5	47,52,52	0.69	1 (2%)	58,81,81	1.18	4 (6%)
12	HEC	K	200	3	46,50,50	1.81	11 (23%)	58,82,82	1.53	11 (18%)
11	PG4	G	2006	-	12,12,12	0.37	0	11,11,11	0.42	0
9	HEM	J	200	3	50,50,50	1.62	6 (12%)	67,82,82	1.54	9 (13%)
4	MGD	C	2002	5	47,52,52	0.59	1 (2%)	58,81,81	1.02	4 (6%)
4	MGD	E	2002	5	47,52,52	0.59	0	58,81,81	1.17	5 (8%)
6	F3S	E	2004	1	0,9,9	-	-	-		
8	FES	B	201	2	0,4,4	-	-	-		
6	F3S	A	2004	1	0,9,9	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MGD	E	2001	5	47,52,52	0.63	1 (2%)	58,81,81	1.00	3 (5%)
4	MGD	C	2001	5	47,52,52	0.52	0	58,81,81	1.04	4 (6%)
8	FES	D	201	2	0,4,4	-	-	-		

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
10	GOL	E	2006	-	-	4/4/4/4	-
8	FES	H	201	2	-	-	0/1/1/1
6	F3S	G	2004	1	-	-	0/3/3/3
4	MGD	G	2001	5	-	4/22/66/66	0/6/6/6
11	PG4	E	2007	-	-	5/10/10/10	-
9	HEM	I	200	3	-	0/14/54/54	-
4	MGD	A	2002	5	-	5/22/66/66	0/6/6/6
9	HEM	L	200	3	-	1/14/54/54	-
8	FES	F	201	2	-	-	0/1/1/1
6	F3S	C	2004	1	-	-	0/3/3/3
4	MGD	G	2002	5	-	5/22/66/66	0/6/6/6
4	MGD	A	2001	5	-	4/22/66/66	0/6/6/6
12	HEC	K	200	3	-	5/14/54/54	-
11	PG4	G	2006	-	-	9/10/10/10	-
9	HEM	J	200	3	-	3/14/54/54	-
4	MGD	C	2002	5	-	5/22/66/66	0/6/6/6
4	MGD	E	2002	5	-	5/22/66/66	0/6/6/6
6	F3S	E	2004	1	-	-	0/3/3/3
8	FES	B	201	2	-	-	0/1/1/1
6	F3S	A	2004	1	-	-	0/3/3/3
4	MGD	E	2001	5	-	4/22/66/66	0/6/6/6
4	MGD	C	2001	5	-	4/22/66/66	0/6/6/6
8	FES	D	201	2	-	-	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	200	HEM	FE-NB	5.66	2.12	1.94
9	J	200	HEM	FE-NB	5.65	2.12	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	200	HEM	FE-NB	4.92	2.10	1.94
9	J	200	HEM	FE-NC	4.88	2.11	1.95
9	L	200	HEM	FE-NC	4.82	2.11	1.95
12	K	200	HEC	CAC-C3C	4.69	1.50	1.35
9	I	200	HEM	FE-NC	4.31	2.09	1.95
12	K	200	HEC	CBB-CAB	-4.22	1.33	1.49
12	K	200	HEC	CBC-CAC	-4.13	1.34	1.49
12	K	200	HEC	CAB-C3B	3.64	1.46	1.35
9	J	200	HEM	C1B-NB	-3.58	1.34	1.40
4	A	2001	MGD	C23-C14	3.31	1.56	1.53
9	I	200	HEM	C4D-ND	-3.17	1.34	1.40
12	K	200	HEC	C1B-NB	-3.12	1.33	1.39
9	L	200	HEM	C4D-ND	-3.02	1.35	1.40
9	I	200	HEM	C1B-NB	-3.00	1.35	1.40
12	K	200	HEC	C1A-C2A	-2.97	1.40	1.45
12	K	200	HEC	C4B-NB	-2.96	1.34	1.39
9	J	200	HEM	C4D-ND	-2.92	1.35	1.40
9	L	200	HEM	C1B-NB	-2.82	1.35	1.40
4	E	2001	MGD	C23-C14	2.78	1.55	1.53
12	K	200	HEC	C1D-ND	-2.53	1.34	1.39
9	I	200	HEM	C4B-NB	-2.45	1.34	1.38
12	K	200	HEC	C4A-C3A	-2.32	1.40	1.45
9	L	200	HEM	C3B-C4B	2.26	1.49	1.44
9	J	200	HEM	C3C-C2C	2.24	1.41	1.37
9	J	200	HEM	C4B-NB	-2.09	1.34	1.38
12	K	200	HEC	C4D-ND	-2.08	1.35	1.39
4	C	2002	MGD	C23-C14	2.06	1.55	1.53
12	K	200	HEC	C1D-C2D	2.04	1.47	1.43
9	I	200	HEM	C1C-NC	-2.03	1.35	1.39

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	200	HEM	CHC-C4B-NB	4.99	129.79	124.42
12	K	200	HEC	CHC-C4B-NB	4.99	129.88	124.45
9	I	200	HEM	CHC-C4B-NB	4.95	129.75	124.42
9	L	200	HEM	CHC-C4B-NB	4.80	129.59	124.42
4	G	2002	MGD	C23-C14-N15	4.60	112.39	107.87
9	L	200	HEM	C1B-NB-C4B	4.26	110.26	105.21
4	A	2001	MGD	C23-C14-N15	3.97	111.77	107.87
9	I	200	HEM	C1B-NB-C4B	3.91	109.84	105.21
9	I	200	HEM	CHD-C1D-ND	3.79	128.50	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	200	HEM	C1B-NB-C4B	3.68	109.56	105.21
4	A	2001	MGD	O11-C23-C14	3.59	111.36	108.96
4	E	2001	MGD	C19-N20-C21	3.48	119.51	113.36
4	A	2001	MGD	C19-N20-C21	3.42	119.39	113.36
4	E	2002	MGD	O11-C23-C14	3.42	111.24	108.96
9	I	200	HEM	CHA-C4D-ND	3.41	128.59	124.37
4	E	2002	MGD	C19-N20-C21	3.35	119.27	113.36
4	E	2002	MGD	C23-C14-N15	3.29	111.10	107.87
4	E	2001	MGD	C23-C14-N15	3.27	111.08	107.87
9	J	200	HEM	CHD-C1D-ND	3.27	127.94	124.42
4	G	2001	MGD	C23-C14-N15	3.26	111.07	107.87
4	A	2002	MGD	C23-C14-N15	3.23	111.04	107.87
4	G	2001	MGD	C19-N20-C21	3.22	119.05	113.36
4	C	2001	MGD	C19-N20-C21	3.22	119.04	113.36
4	G	2002	MGD	C19-N20-C21	3.09	118.80	113.36
9	J	200	HEM	CHA-C4D-ND	3.03	128.11	124.37
9	L	200	HEM	C3B-C4B-NB	-2.99	107.32	109.47
9	I	200	HEM	CHD-C1D-C2D	-2.99	120.30	125.03
9	J	200	HEM	CHB-C1B-NB	2.99	128.07	124.37
9	L	200	HEM	CHD-C1D-ND	2.99	127.64	124.42
12	K	200	HEC	O2D-CGD-CBD	2.87	123.08	114.00
4	A	2002	MGD	C19-N20-C21	2.84	118.37	113.36
9	I	200	HEM	CBD-CAD-C3D	-2.84	104.69	112.53
12	K	200	HEC	CHA-C1A-NA	2.82	127.53	124.45
9	L	200	HEM	CHA-C4D-ND	2.71	127.72	124.37
4	C	2001	MGD	C23-C14-N15	2.71	110.53	107.87
4	C	2002	MGD	C19-N20-C21	2.71	118.14	113.36
4	A	2002	MGD	C4'-O4'-C1'	-2.67	103.57	109.47
4	A	2002	MGD	O11-C23-C14	2.63	110.72	108.96
4	C	2002	MGD	C4'-O4'-C1'	-2.55	103.83	109.47
4	G	2002	MGD	C4'-O4'-C1'	-2.55	103.83	109.47
4	G	2001	MGD	O11-C23-C14	2.55	110.66	108.96
4	C	2002	MGD	O11-C23-N22	2.52	110.89	108.61
9	J	200	HEM	CHD-C1D-C2D	-2.51	121.07	125.03
9	I	200	HEM	CHB-C1B-NB	2.48	127.43	124.37
4	G	2001	MGD	C17-C16-N15	2.47	123.01	116.27
12	K	200	HEC	CHD-C1D-ND	2.46	128.32	123.86
12	K	200	HEC	CHB-C1B-NB	2.45	128.30	123.86
12	K	200	HEC	CBB-CAB-C3B	-2.44	122.56	127.43
9	L	200	HEM	CHB-C1B-NB	2.42	127.36	124.37
4	E	2002	MGD	O3B-PB-O1B	-2.42	103.43	110.70
12	K	200	HEC	CHD-C1D-C2D	-2.41	120.43	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	200	HEM	CHD-C1D-C2D	-2.40	121.24	125.03
4	E	2001	MGD	C17-C16-N15	2.40	122.81	116.27
12	K	200	HEC	CBA-CAA-C2A	-2.40	105.91	112.53
9	L	200	HEM	CHD-C4C-NC	2.39	127.06	124.45
9	J	200	HEM	C3B-C4B-NB	-2.37	107.76	109.47
4	C	2001	MGD	O2B-PB-O3B	2.37	113.67	107.27
9	J	200	HEM	O2A-CGA-CBA	2.33	121.36	114.00
9	L	200	HEM	CBD-CAD-C3D	-2.32	106.11	112.53
9	J	200	HEM	CHA-C4D-C3D	-2.32	120.94	125.23
4	A	2001	MGD	C17-C16-N15	2.31	122.56	116.27
4	C	2002	MGD	O3B-PB-O1B	-2.26	103.90	110.70
9	I	200	HEM	C3B-C4B-NB	-2.19	107.89	109.47
9	I	200	HEM	CHD-C4C-NC	2.17	126.81	124.45
4	C	2001	MGD	C17-C16-N15	2.16	122.16	116.27
9	L	200	HEM	C2A-C1A-NA	-2.15	107.77	110.15
9	L	200	HEM	O2A-CGA-O1A	-2.12	117.87	123.33
4	G	2002	MGD	O11-C23-C14	2.11	110.37	108.96
12	K	200	HEC	C4B-NB-C1B	2.11	109.25	105.82
4	G	2002	MGD	O2A-PA-O1A	2.10	122.23	112.44
4	E	2002	MGD	C4'-O4'-C1'	-2.10	104.84	109.47
12	K	200	HEC	C2A-C1A-NA	-2.09	108.30	110.32
9	I	200	HEM	C1A-CHA-C4D	-2.06	121.40	126.25
4	A	2002	MGD	C17-C16-N15	2.06	121.89	116.27
12	K	200	HEC	CBD-CAD-C3D	-2.06	106.84	112.53
9	L	200	HEM	O2D-CGD-CBD	2.05	120.47	114.00
9	L	200	HEM	CBA-CAA-C2A	-2.02	106.95	112.53
9	L	200	HEM	CHA-C1A-NA	2.01	127.51	123.86

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2001	MGD	C5'-O5'-PB-O3B
4	A	2002	MGD	PA-O3B-PB-O5'
4	A	2002	MGD	C5'-O5'-PB-O1B
4	A	2002	MGD	C5'-O5'-PB-O3B
4	C	2001	MGD	C5'-O5'-PB-O3B
4	C	2002	MGD	C5'-O5'-PB-O1B
4	C	2002	MGD	C5'-O5'-PB-O3B
4	E	2001	MGD	PA-O3B-PB-O5'
4	E	2001	MGD	C5'-O5'-PB-O3B
4	E	2002	MGD	C5'-O5'-PB-O1B

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Mol	Chain	Res	Type	Atoms
4	G	2001	MGD	PA-O3B-PB-O5'
4	G	2001	MGD	C5'-O5'-PB-O3B
4	G	2002	MGD	C5'-O5'-PB-O1B
4	G	2002	MGD	C5'-O5'-PB-O3B
12	K	200	HEC	C2B-C3B-CAB-CBB
12	K	200	HEC	C4B-C3B-CAB-CBB
11	G	2006	PG4	C1-C2-O2-C3
11	G	2006	PG4	C8-C7-O4-C6
11	G	2006	PG4	O2-C3-C4-O3
11	G	2006	PG4	O3-C5-C6-O4
11	E	2007	PG4	O4-C7-C8-O5
10	E	2006	GOL	O1-C1-C2-C3
10	E	2006	GOL	C1-C2-C3-O3
11	G	2006	PG4	O1-C1-C2-O2
10	E	2006	GOL	O1-C1-C2-O2
10	E	2006	GOL	O2-C2-C3-O3
11	G	2006	PG4	O4-C7-C8-O5
12	K	200	HEC	C3D-CAD-CBD-CGD
11	E	2007	PG4	O1-C1-C2-O2
11	E	2007	PG4	O3-C5-C6-O4
4	A	2001	MGD	PA-O3B-PB-O5'
4	C	2001	MGD	PA-O3B-PB-O5'
4	C	2002	MGD	PA-O3B-PB-O5'
4	E	2002	MGD	PA-O3B-PB-O5'
4	G	2002	MGD	PA-O3B-PB-O5'
11	E	2007	PG4	C8-C7-O4-C6
9	J	200	HEM	C2A-CAA-CBA-CGA
11	G	2006	PG4	C5-C6-O4-C7
11	E	2007	PG4	C5-C6-O4-C7
11	G	2006	PG4	C6-C5-O3-C4
11	G	2006	PG4	C4-C3-O2-C2
4	A	2001	MGD	C5'-O5'-PB-O1B
4	A	2001	MGD	C10-O3A-PA-O1A
4	A	2002	MGD	C5'-O5'-PB-O2B
4	C	2001	MGD	C5'-O5'-PB-O1B
4	C	2002	MGD	C5'-O5'-PB-O2B
4	E	2001	MGD	C5'-O5'-PB-O1B
4	E	2002	MGD	C5'-O5'-PB-O2B
4	E	2002	MGD	C5'-O5'-PB-O3B
4	G	2001	MGD	C5'-O5'-PB-O1B
4	G	2001	MGD	C10-O3A-PA-O1A
4	G	2002	MGD	C5'-O5'-PB-O2B

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Mol	Chain	Res	Type	Atoms
9	L	200	HEM	C3D-CAD-CBD-CGD
4	C	2001	MGD	O4'-C4'-C5'-O5'
9	J	200	HEM	C3D-CAD-CBD-CGD
4	E	2001	MGD	O4'-C4'-C5'-O5'
12	K	200	HEC	CAD-CBD-CGD-O1D
12	K	200	HEC	CAD-CBD-CGD-O2D
9	J	200	HEM	CAA-CBA-CGA-O2A
4	A	2002	MGD	PB-O3B-PA-O2A
4	C	2002	MGD	PB-O3B-PA-O2A
4	E	2002	MGD	PB-O3B-PA-O2A
4	G	2002	MGD	PB-O3B-PA-O2A

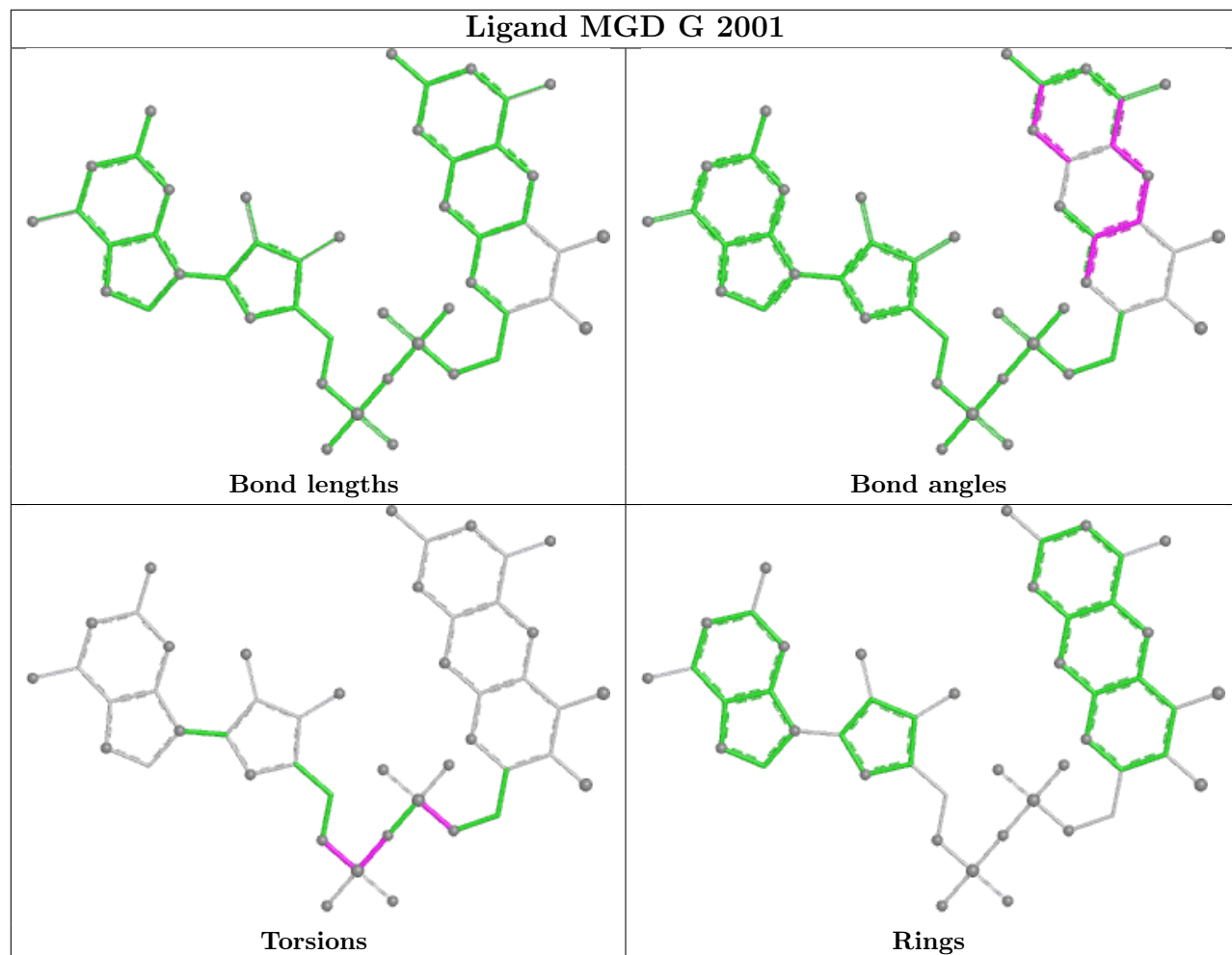
There are no ring outliers.

14 monomers are involved in 66 short contacts:

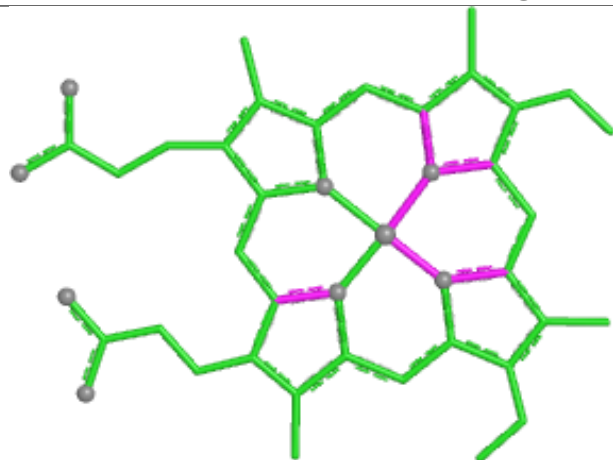
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	E	2006	GOL	1	0
4	G	2001	MGD	1	0
9	I	200	HEM	9	0
4	A	2002	MGD	2	0
9	L	200	HEM	10	0
6	C	2004	F3S	1	0
4	G	2002	MGD	1	0
12	K	200	HEC	5	0
11	G	2006	PG4	20	0
9	J	200	HEM	10	0
4	C	2002	MGD	1	0
4	E	2001	MGD	2	0
4	C	2001	MGD	2	0
8	D	201	FES	1	0

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

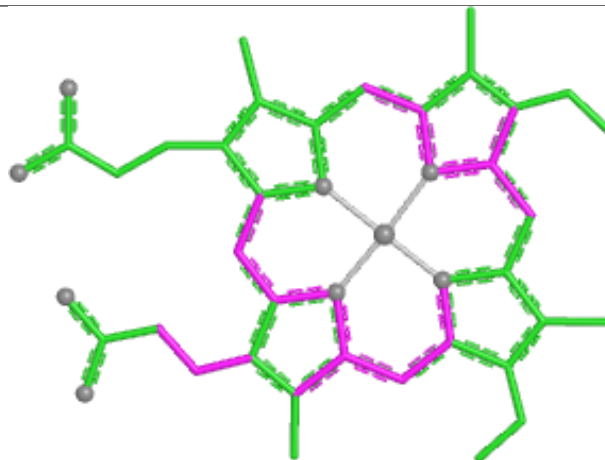
equivalents in the CSD to analyse the geometry.



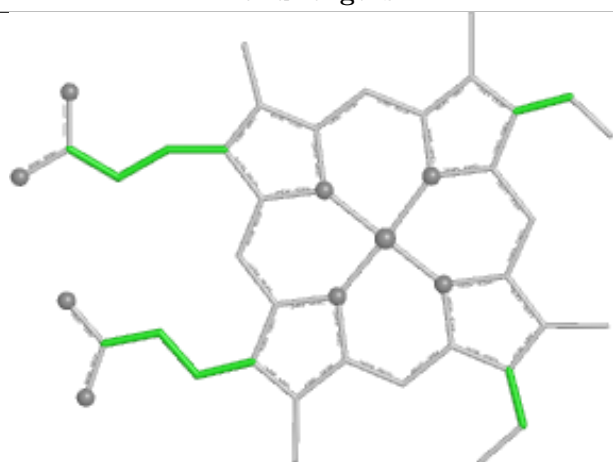
Ligand HEM I 200



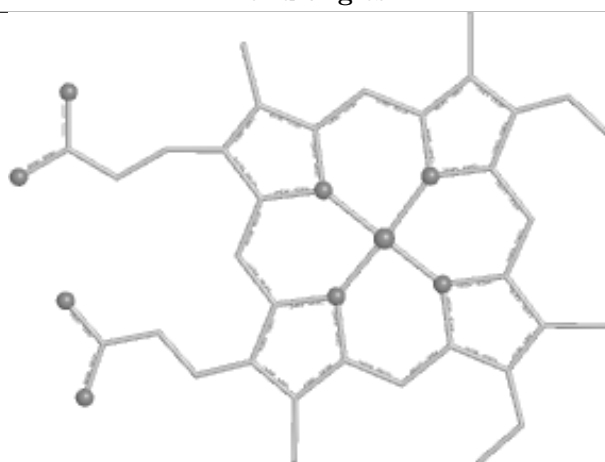
Bond lengths



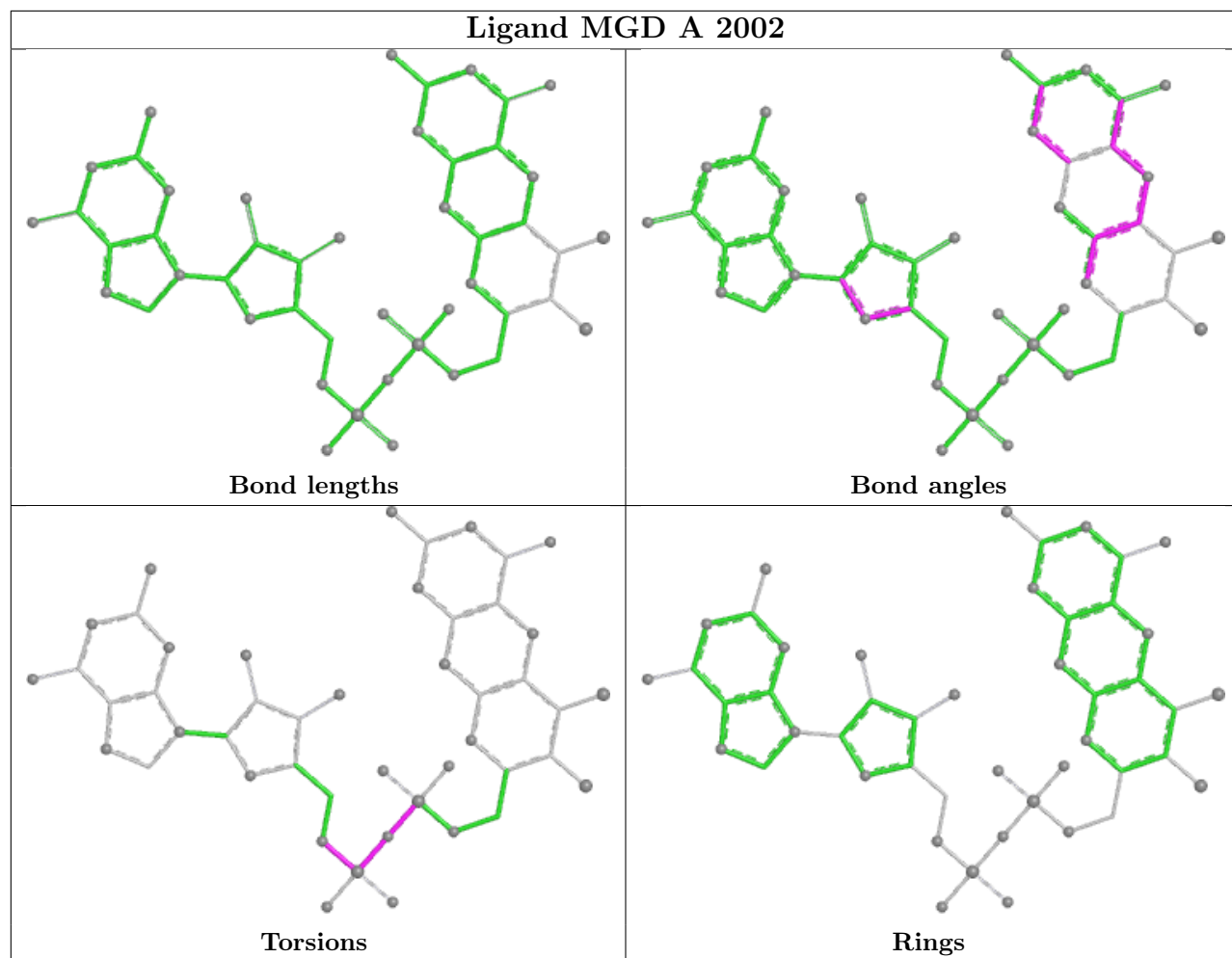
Bond angles

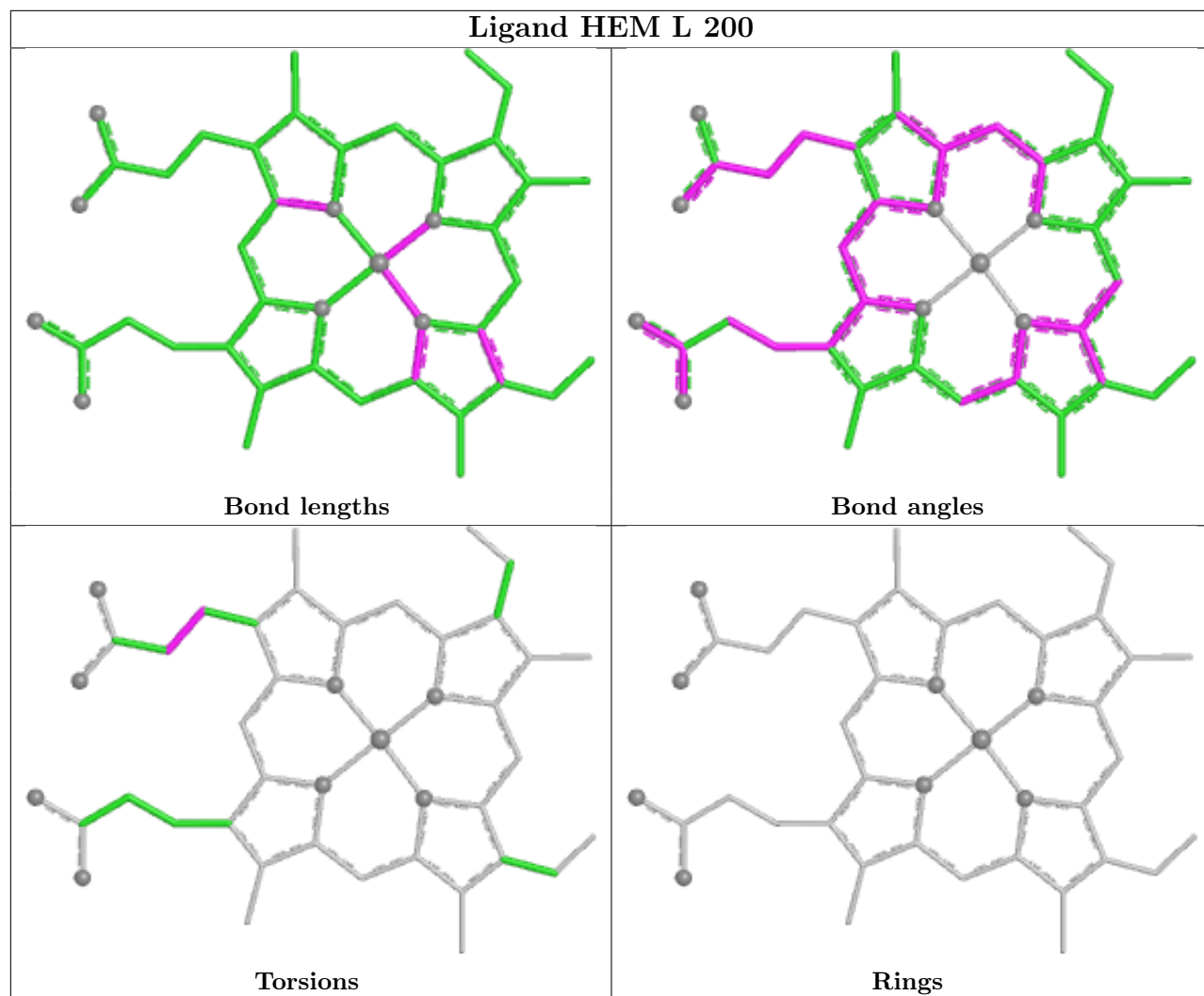


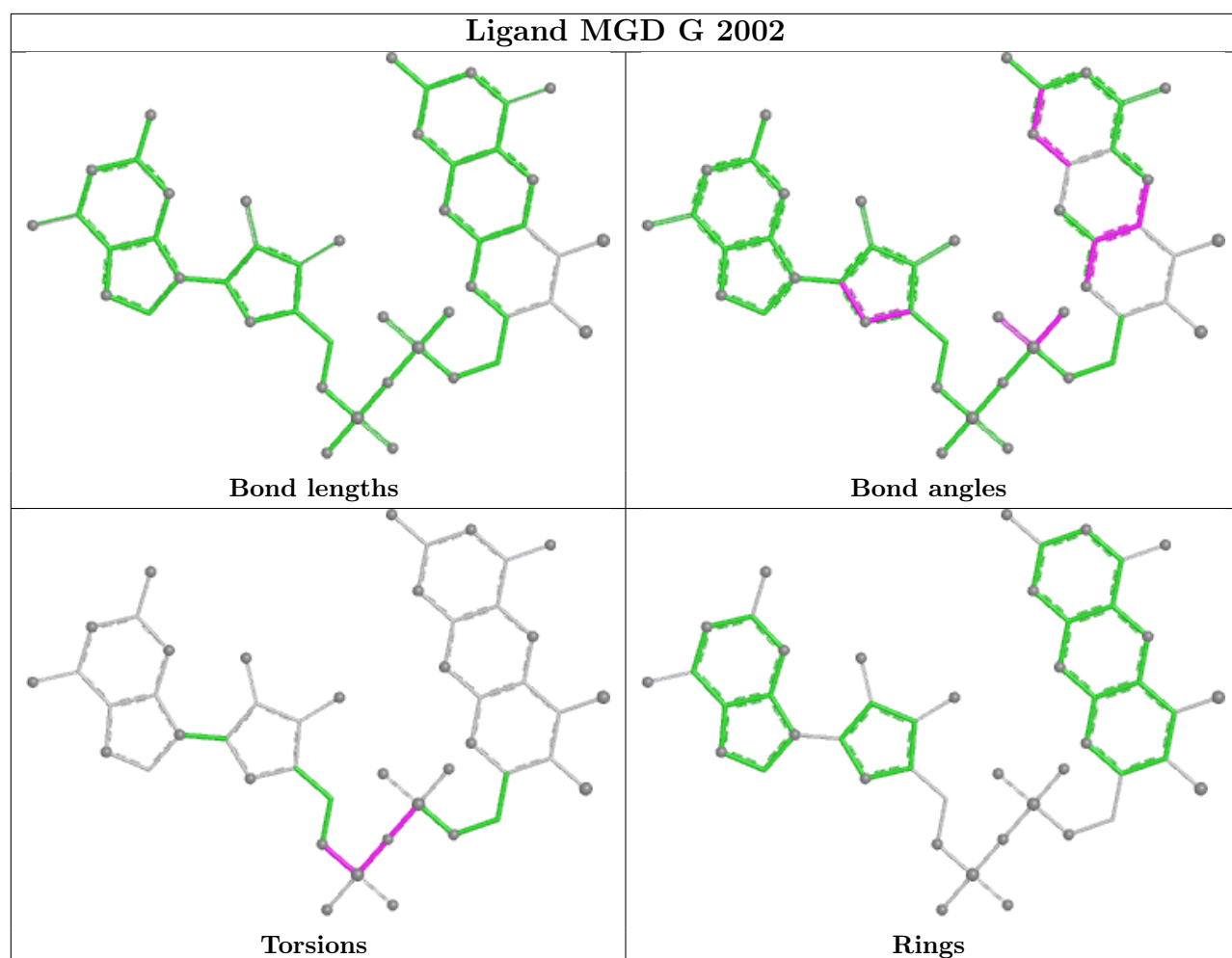
Torsions

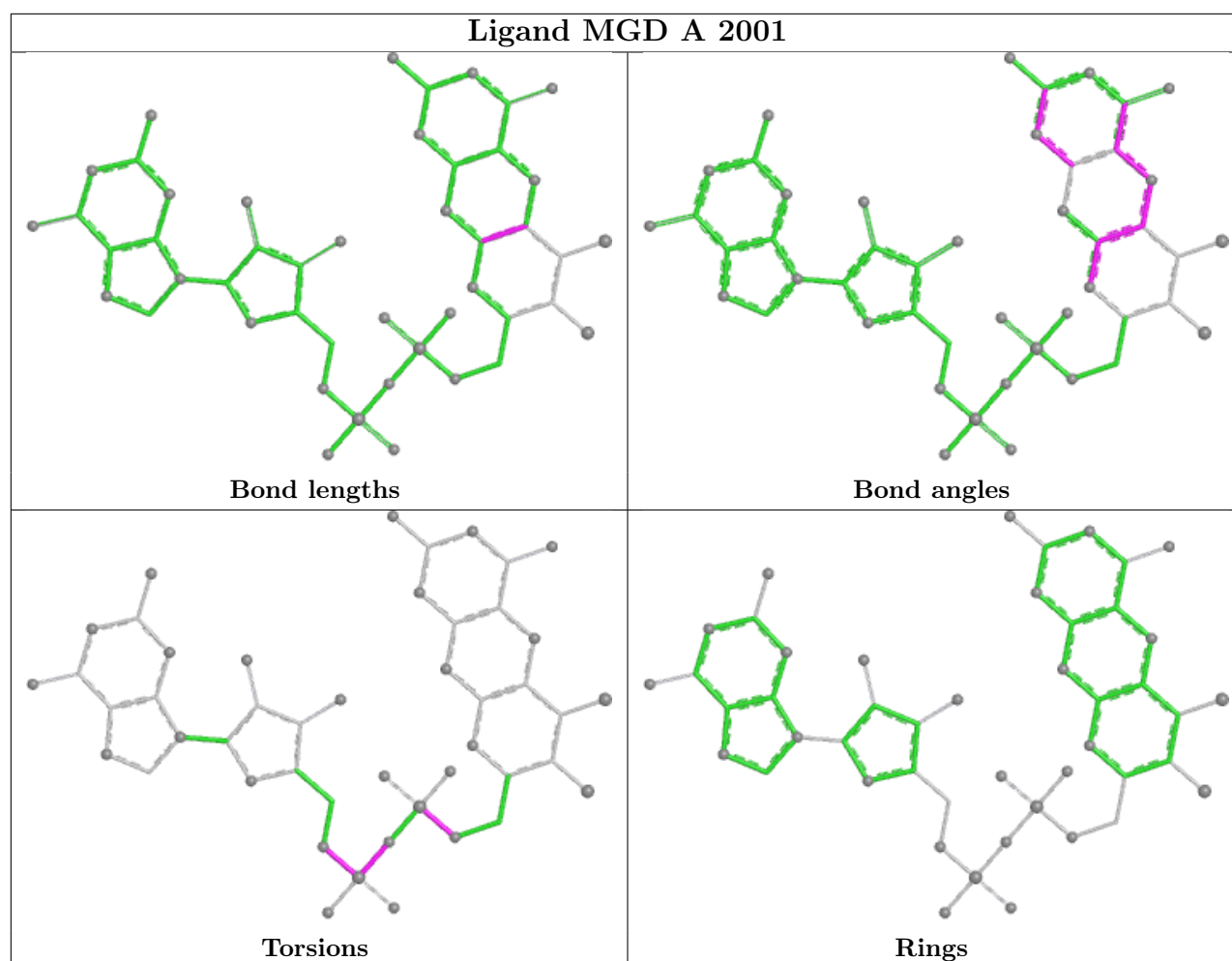


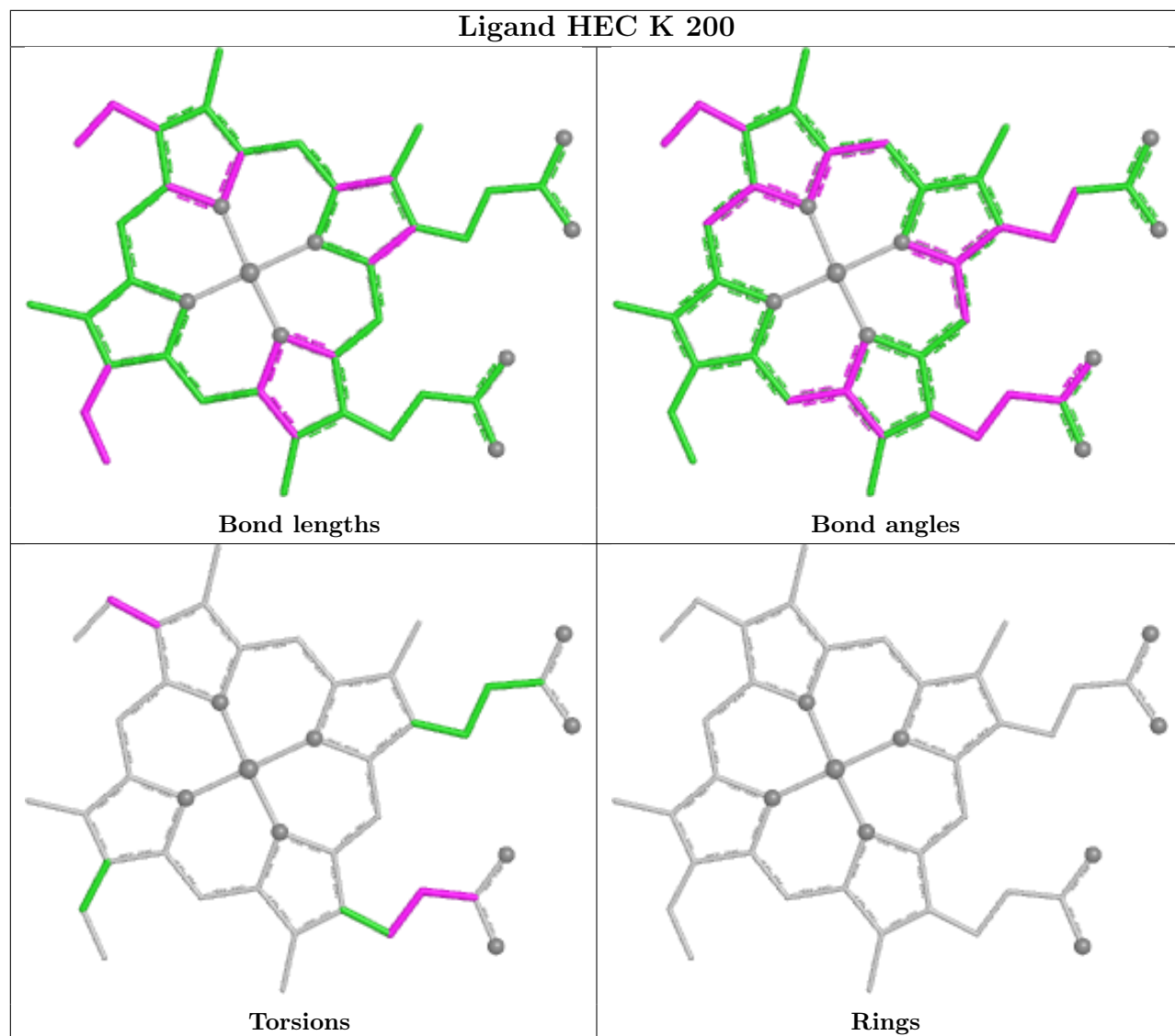
Rings

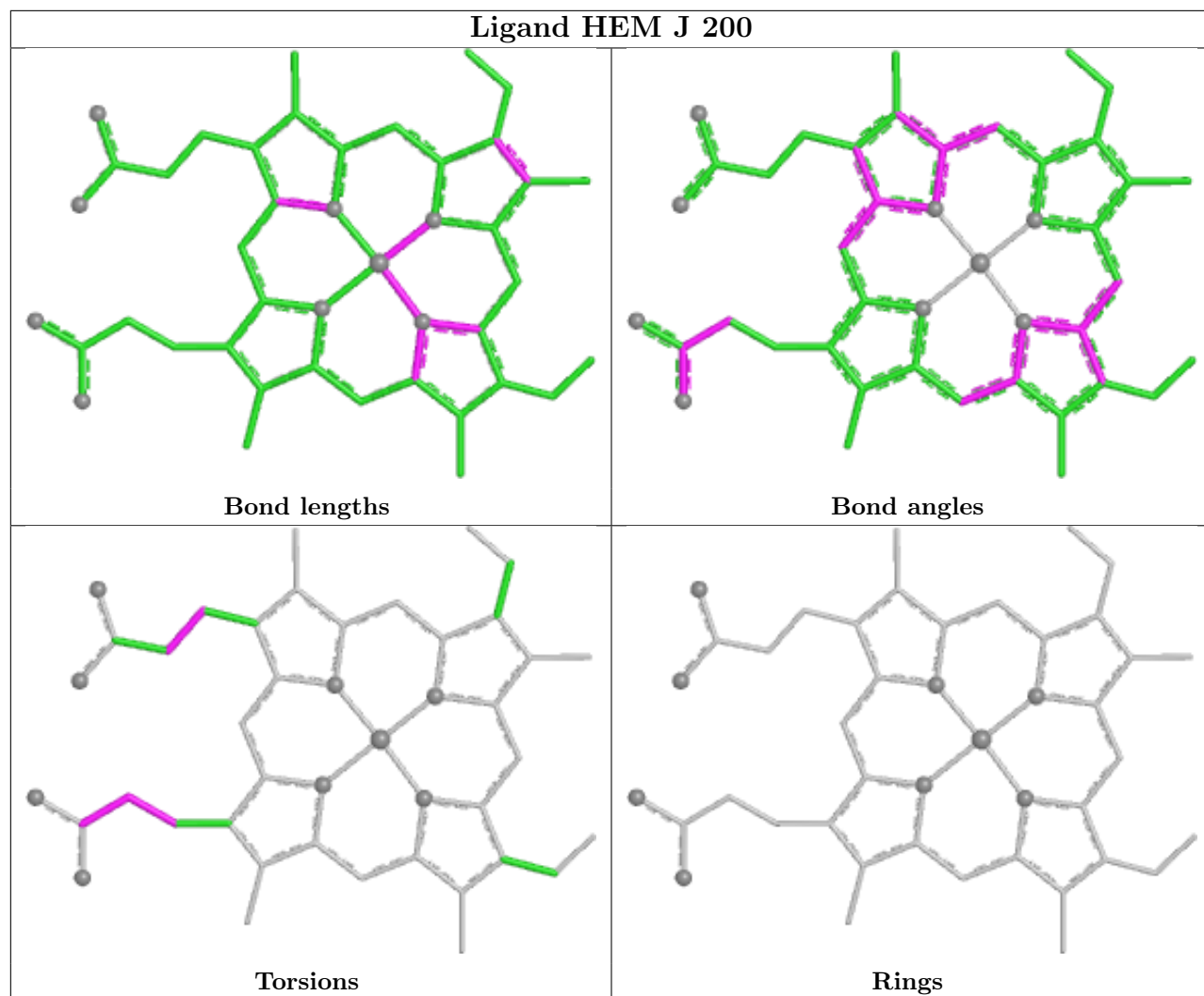


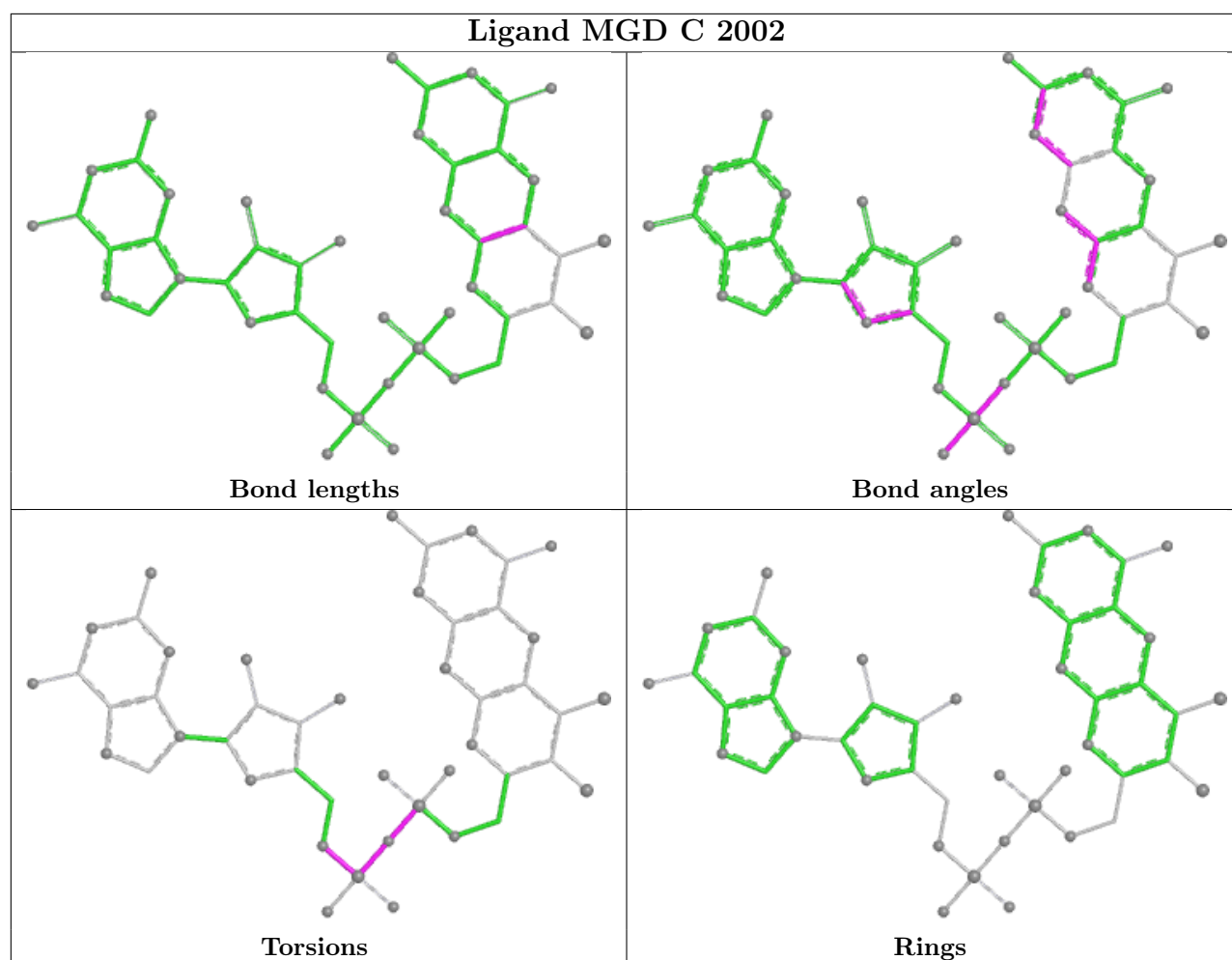


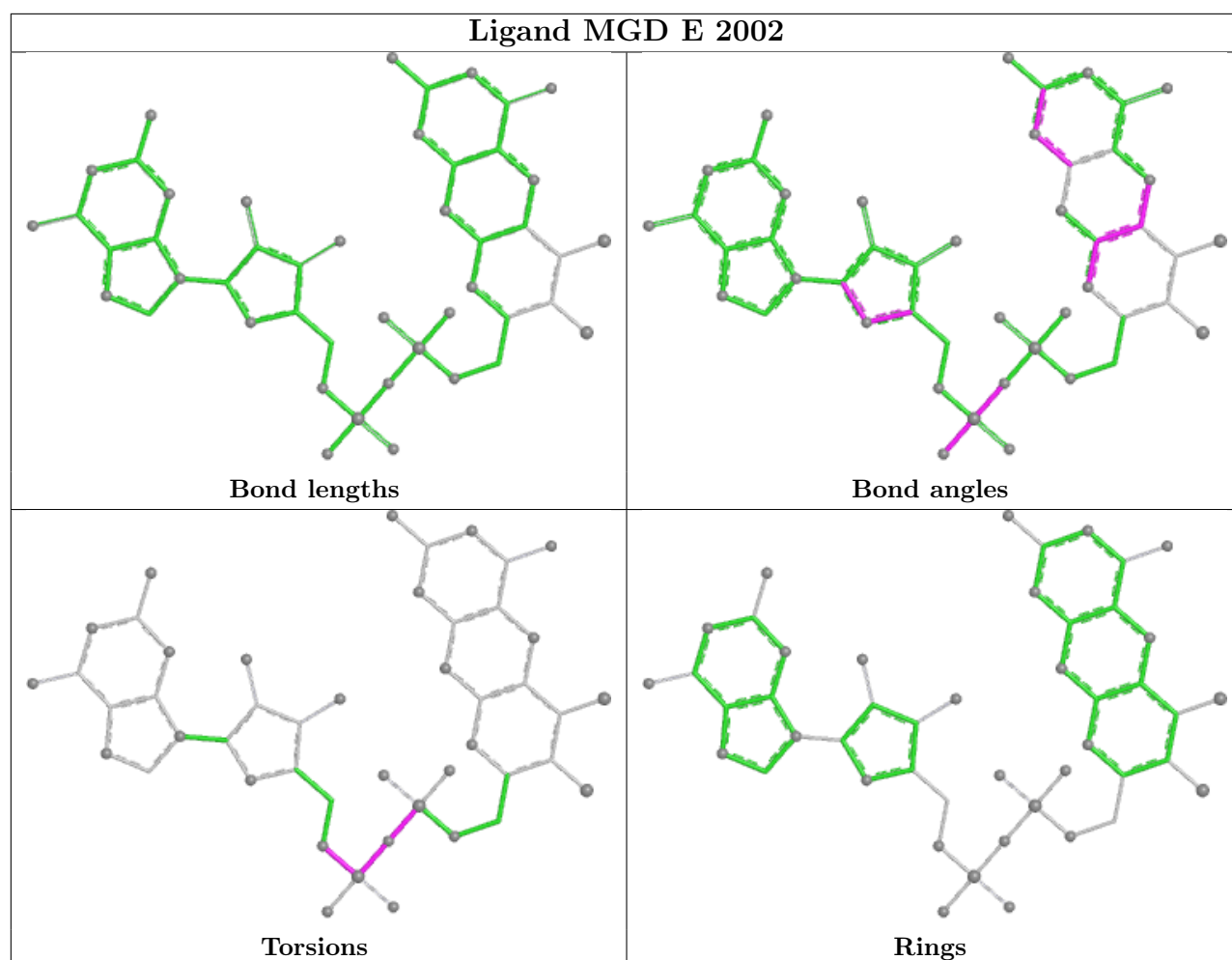


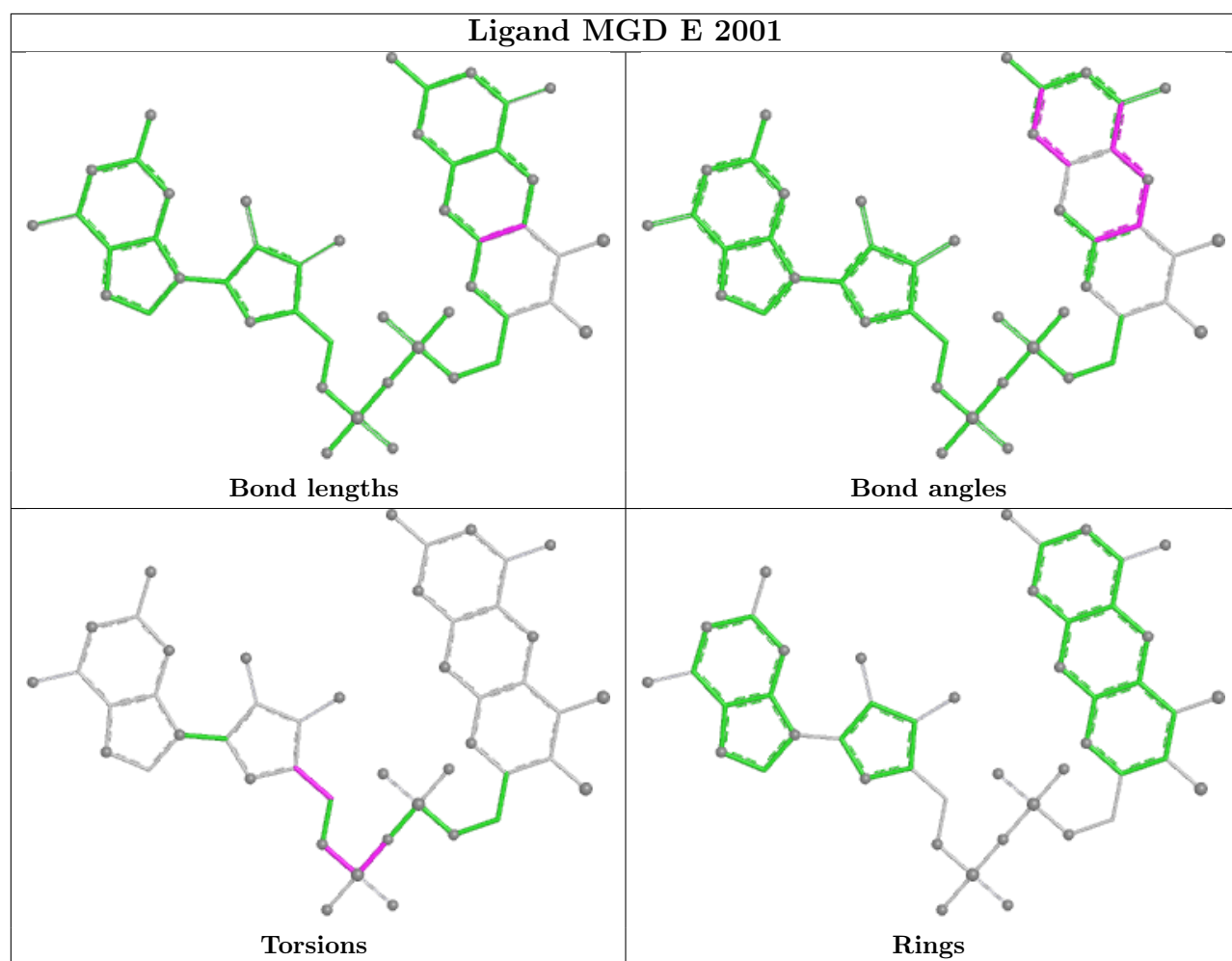


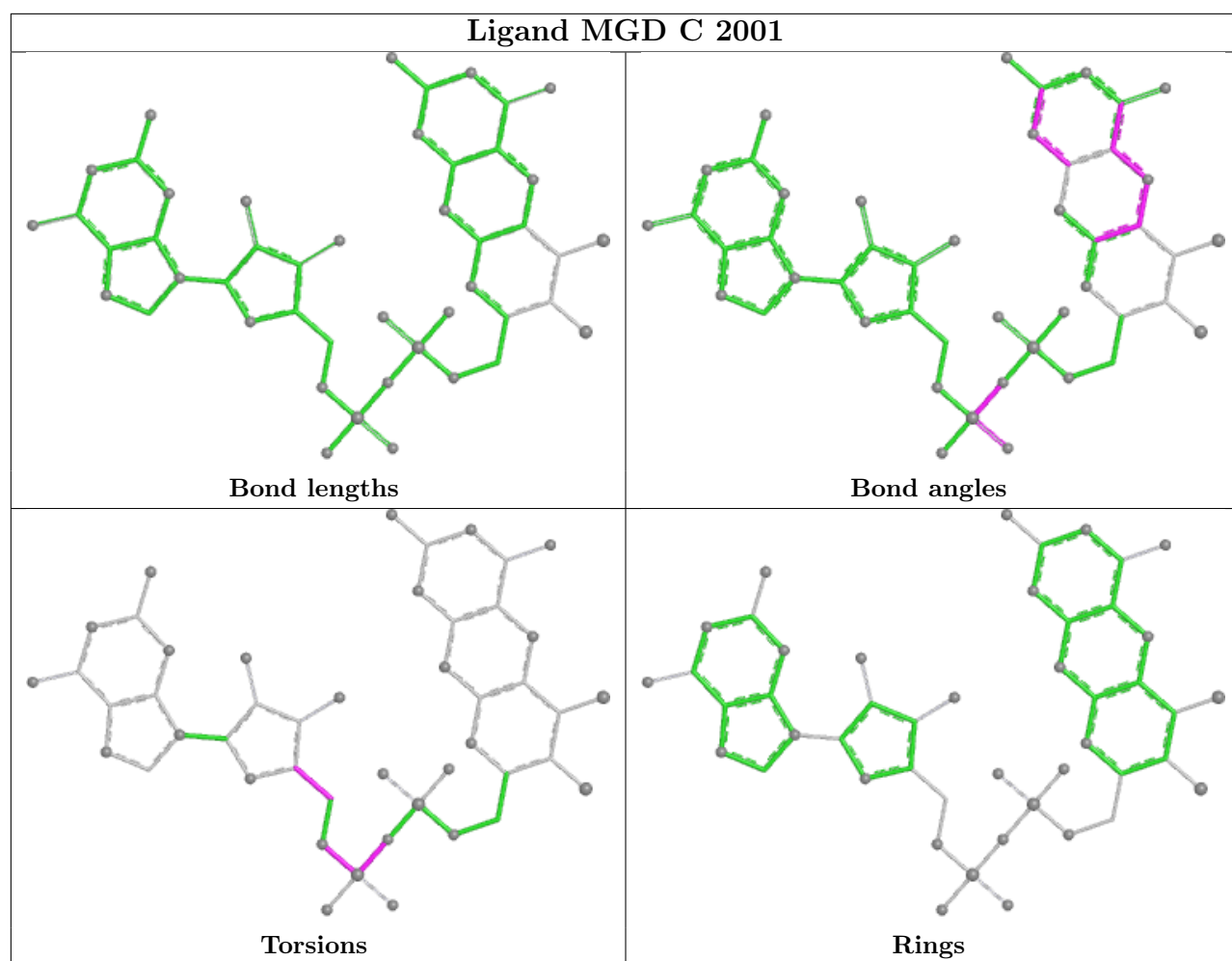












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	843/844 (99%)	0.07	17 (2%) 65 65	0, 8, 27, 50	5 (0%)
1	C	843/844 (99%)	0.11	17 (2%) 65 65	0, 10, 27, 46	5 (0%)
1	E	843/844 (99%)	-0.20	4 (0%) 87 88	0, 4, 18, 35	12 (1%)
1	G	843/844 (99%)	-0.26	3 (0%) 88 89	0, 1, 16, 38	9 (1%)
2	B	132/162 (81%)	0.60	4 (3%) 52 53	5, 20, 39, 47	0
2	D	132/162 (81%)	1.38	34 (25%) 1 1	11, 24, 43, 51	0
2	F	132/162 (81%)	-0.01	1 (0%) 82 84	1, 9, 17, 28	0
2	H	131/162 (80%)	-0.06	0 100 100	1, 10, 18, 25	0
3	I	105/117 (89%)	1.98	43 (40%) 0 0	15, 37, 57, 67	0
3	J	102/117 (87%)	3.62	90 (88%) 0 0	23, 57, 85, 103	0
3	K	103/117 (88%)	2.18	49 (47%) 0 0	17, 40, 63, 81	0
3	L	102/117 (87%)	2.15	55 (53%) 0 0	20, 40, 60, 62	1 (0%)
All	All	4311/4492 (95%)	0.24	317 (7%) 20 19	0, 8, 43, 103	32 (0%)

All (317) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	96	ALA	8.0
3	J	55	LEU	7.5
3	J	85	VAL	7.2
3	J	74	ALA	6.8
3	J	80	TRP	6.6
3	K	124	PHE	6.4
3	J	56	ILE	6.3
3	J	81	VAL	6.1
3	K	105	PHE	5.9
3	I	24	ALA	5.9
3	J	61	ALA	5.8

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Mol	Chain	Res	Type	RSRZ
3	L	25[A]	GLU	5.7
3	J	104	ALA	5.6
3	K	104	ALA	5.4
3	I	85	VAL	5.4
3	I	105	PHE	5.4
3	K	80	TRP	5.4
3	J	43	GLY	5.4
3	J	121	LEU	5.4
3	J	54	GLY	5.3
3	L	29	VAL	5.3
3	I	80	TRP	5.3
3	J	98	ILE	5.2
3	J	97	TYR	5.2
3	J	87	LEU	5.0
3	J	105	PHE	5.0
3	J	124	PHE	5.0
3	J	57	GLY	5.0
3	K	22	SER	4.9
3	K	81	VAL	4.9
3	J	108	LEU	4.9
3	J	26	LYS	4.8
3	L	45	ALA	4.8
3	L	119	ALA	4.7
3	J	83	ASP	4.7
3	L	40	VAL	4.6
3	I	86	HIS	4.6
3	J	70	PRO	4.6
3	L	124	PHE	4.5
3	J	106	ALA	4.5
3	J	115	ALA	4.5
3	K	76	ALA	4.5
3	J	73	LYS	4.5
1	C	268	PRO	4.5
3	J	88	THR	4.5
3	J	86	HIS	4.5
3	I	99	LYS	4.4
3	J	79	GLY	4.4
3	I	126	THR	4.4
3	K	123	THR	4.4
3	J	71	ALA	4.4
3	J	41	GLY	4.4
3	L	64	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
3	J	111	PRO	4.3
3	J	82	TRP	4.3
3	K	79	GLY	4.3
3	I	104	ALA	4.3
3	L	104	ALA	4.2
3	L	24	ALA	4.2
2	D	57	ILE	4.1
3	K	122	LYS	4.1
3	L	23	ASN	4.1
3	I	106	ALA	4.0
3	J	76	ALA	4.0
3	L	56	ILE	4.0
3	J	102	LYS	3.9
3	J	114	VAL	3.9
3	J	117	VAL	3.9
1	C	668	ASP	3.9
3	L	43	GLY	3.9
3	J	113	ASP	3.9
3	J	60	VAL	3.9
3	J	28	ALA	3.9
3	J	42	ASP	3.9
3	I	125	SER	3.8
3	J	78	GLU	3.8
2	B	57	ILE	3.8
3	J	92	ALA	3.8
3	J	64	GLU	3.8
2	D	156	GLY	3.8
3	J	75	LYS	3.7
3	J	58	ARG	3.7
3	J	49	GLY	3.7
3	J	95	LYS	3.7
3	J	90	TYR	3.7
3	L	120	TYR	3.7
3	J	59	LYS	3.7
2	D	153	ALA	3.6
3	K	74	ALA	3.6
3	J	120	TYR	3.6
3	J	25	GLU	3.6
3	J	77	GLU	3.6
3	K	85	VAL	3.6
3	L	30	VAL	3.6
3	J	24	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
3	J	52	LEU	3.6
3	K	82	TRP	3.6
3	K	106	ALA	3.6
3	K	59	LYS	3.6
3	L	123	THR	3.6
3	I	97	TYR	3.5
3	J	72	PHE	3.5
3	L	109	LYS	3.5
3	K	24	ALA	3.5
1	A	41	ASN	3.5
3	I	112	GLU	3.5
3	K	97	TYR	3.5
3	L	65	GLY	3.4
3	J	109	LYS	3.4
3	J	107	GLY	3.4
3	J	110	LYS	3.4
3	I	111	PRO	3.4
2	D	46	GLY	3.4
1	C	46	THR	3.3
2	D	89	GLY	3.3
3	L	44	ALA	3.3
3	J	23	ASN	3.3
2	D	91	GLY	3.3
3	J	122	LYS	3.3
3	L	110	LYS	3.3
3	K	23	ASN	3.2
3	L	31	PHE	3.2
2	D	44	ALA	3.2
1	C	340	GLY	3.2
3	I	113	ASP	3.2
3	K	86	HIS	3.2
3	K	57	GLY	3.2
3	I	98	ILE	3.2
1	A	339	GLU	3.2
3	J	84	GLU	3.2
3	L	54	GLY	3.2
3	I	70	PRO	3.2
1	A	40	ILE	3.2
3	L	118	ILE	3.2
3	J	101	THR	3.2
3	J	62	GLY	3.1
3	J	119	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
3	K	96	ALA	3.1
1	A	614	VAL	3.1
3	J	99	LYS	3.1
3	I	88	THR	3.1
3	K	72	PHE	3.1
1	A	340	GLY	3.1
3	L	28	ALA	3.1
3	J	63	VAL	3.1
3	J	31	PHE	3.1
3	J	100	GLY	3.1
3	L	36	ALA	3.1
3	I	114	VAL	3.1
3	L	48	VAL	3.1
3	J	53	ASN	3.0
3	I	115	ALA	3.0
3	K	71	ALA	3.0
3	K	77	GLU	3.0
3	K	26	LYS	3.0
3	K	73	LYS	3.0
3	L	27	GLY	3.0
3	I	109	LYS	3.0
3	J	112	GLU	3.0
3	K	64	GLU	3.0
3	L	35	ALA	2.9
3	L	50	PRO	2.9
1	C	400	GLU	2.9
2	B	92	PRO	2.9
3	K	70	PRO	2.9
3	L	111	PRO	2.9
2	D	152	VAL	2.9
3	L	63	VAL	2.9
1	A	844	SER	2.8
2	D	62	LEU	2.8
3	J	91	LEU	2.8
3	L	85	VAL	2.8
3	I	25	GLU	2.8
3	L	34	CYS	2.8
1	G	340	GLY	2.8
3	L	39	ALA	2.8
1	C	844	SER	2.8
3	I	108	LEU	2.8
3	L	122	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	401	GLY	2.8
1	C	92	HIS	2.7
2	D	158	ILE	2.7
3	J	118	ILE	2.7
3	K	56	ILE	2.7
3	L	42	ASP	2.7
3	J	69	SER	2.7
2	D	54	LEU	2.7
2	D	51	ALA	2.7
2	D	86	VAL	2.7
1	E	41	ASN	2.7
2	B	152	VAL	2.7
3	J	29	VAL	2.7
3	K	60	VAL	2.7
1	A	341	THR	2.7
3	K	42	ASP	2.7
3	J	89	GLU	2.7
3	K	65	GLY	2.7
3	J	44	ALA	2.6
3	J	51	GLU	2.6
3	I	116	ASP	2.6
3	K	121	LEU	2.6
3	J	34	CYS	2.6
3	L	32	LYS	2.6
3	L	108	LEU	2.5
2	D	85	ARG	2.5
1	A	624	ASP	2.5
3	I	82	TRP	2.5
1	C	641	HIS	2.5
2	D	81	LYS	2.5
3	K	95	LYS	2.5
1	A	617	ALA	2.5
2	D	160	ALA	2.5
2	D	65	PRO	2.5
2	D	92	PRO	2.5
3	J	66	PHE	2.5
3	I	81	VAL	2.5
2	D	56	ASN	2.5
3	I	23	ASN	2.5
3	L	26	LYS	2.5
3	I	27	GLY	2.5
1	C	265	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
3	J	103	MET	2.5
3	K	67	ASN	2.5
1	A	342	ALA	2.5
1	A	400	GLU	2.4
3	K	78	GLU	2.4
3	L	112	GLU	2.4
3	I	43	GLY	2.4
3	J	50	PRO	2.4
2	D	68	VAL	2.4
3	J	48	VAL	2.4
2	D	49	TYR	2.4
1	A	47	ASP	2.4
1	C	757	GLY	2.4
2	B	44	ALA	2.4
3	I	96	ALA	2.4
3	K	61	ALA	2.4
2	D	90	VAL	2.4
3	J	30	VAL	2.4
3	K	63	VAL	2.4
3	J	68	TYR	2.4
2	F	154	ASP	2.4
1	A	268	PRO	2.4
3	J	94	PRO	2.4
3	I	107	GLY	2.4
3	J	39	ALA	2.4
3	L	107	GLY	2.4
2	D	58	SER	2.4
3	K	58	ARG	2.4
1	E	340	GLY	2.3
3	J	65	GLY	2.3
3	L	115	ALA	2.3
2	D	84	THR	2.3
2	D	60	LEU	2.3
3	I	67	ASN	2.3
3	L	46	ASN	2.3
3	L	33	LYS	2.3
3	I	28	ALA	2.3
2	D	157	ASP	2.3
3	K	100	GLY	2.3
1	G	92	HIS	2.3
3	I	87	LEU	2.3
2	D	116	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	616	TYR	2.3
1	C	339	GLU	2.3
2	D	96	ILE	2.3
3	I	121	LEU	2.2
3	L	117	VAL	2.3
3	K	107	GLY	2.2
3	I	84	GLU	2.2
3	I	123	THR	2.2
1	G	844	SER	2.2
3	L	95	LYS	2.2
3	K	108	LEU	2.2
2	D	122	PRO	2.2
3	I	26	LYS	2.2
2	D	70	TYR	2.2
1	C	8	ASP	2.2
2	D	73	GLU	2.2
3	K	84	GLU	2.2
3	L	106	ALA	2.2
3	I	66	PHE	2.2
3	J	93	ASN	2.2
3	L	66	PHE	2.2
3	I	77	GLU	2.2
3	L	57	GLY	2.2
1	E	347	TYR	2.1
3	K	90	TYR	2.1
3	J	116	ASP	2.1
3	K	83	ASP	2.1
3	L	114	VAL	2.1
2	D	64	GLU	2.1
3	L	47	LYS	2.1
3	J	27	GLY	2.1
3	I	122	LYS	2.1
3	I	42	ASP	2.1
3	I	74	ALA	2.1
3	L	52	LEU	2.1
1	E	668	ASP	2.1
3	I	29	VAL	2.1
3	K	29	VAL	2.1
1	C	402	GLY	2.1
3	L	62	GLY	2.1
1	C	49	GLN	2.1
2	D	66	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	L	121	LEU	2.1
3	L	41	GLY	2.1
1	C	264	LYS	2.0
1	C	379	GLU	2.0
3	K	119	ALA	2.0
2	D	95	ASP	2.0
3	L	55	LEU	2.0
3	K	117	VAL	2.0
1	A	618	ALA	2.0
1	A	49	GLN	2.0
1	A	333	ASP	2.0
3	K	87	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	PG4	G	2006	13/13	0.73	0.27	0,0,0,0	13
11	PG4	E	2007	13/13	0.79	0.20	12,21,31,34	0
9	HEM	J	200	43/43	0.84	0.18	37,41,44,45	0
10	GOL	E	2006	6/6	0.85	0.19	0,0,0,0	6
9	HEM	I	200	43/43	0.89	0.14	24,27,29,29	0
9	HEM	L	200	43/43	0.91	0.12	22,29,34,36	0
12	HEC	K	200	43/43	0.92	0.12	18,20,22,23	0
7	O	A	2005	1/1	0.95	0.21	30,30,30,30	0
8	FES	D	201	4/4	0.96	0.05	11,13,14,14	0
7	O	C	2005	1/1	0.97	0.19	30,30,30,30	0
7	O	E	2005	1/1	0.97	0.17	30,30,30,30	0

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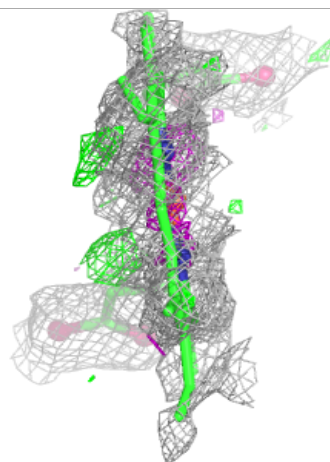
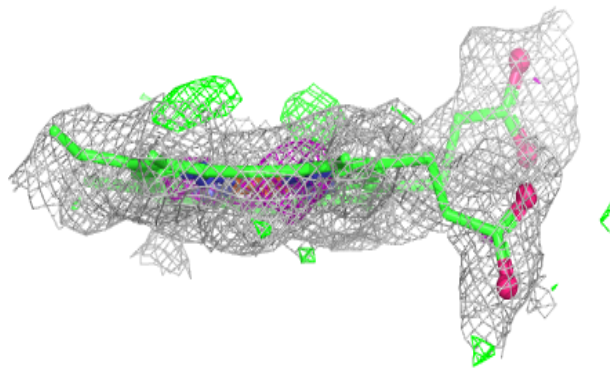
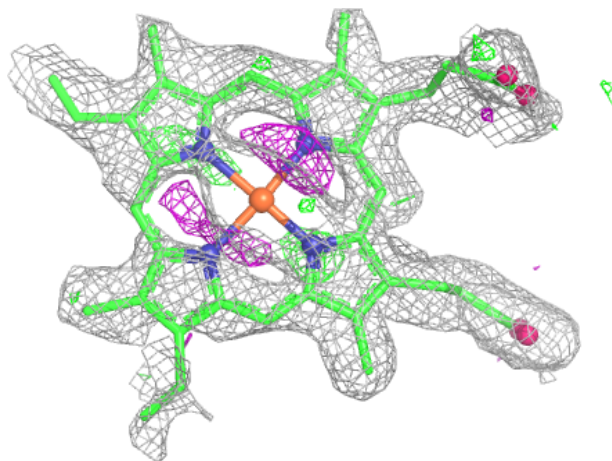
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MGD	C	2002	47/47	0.97	0.06	3,4,4,4	0
6	F3S	A	2004	7/7	0.97	0.05	2,2,2,2	0
4	MGD	A	2001	47/47	0.97	0.06	0,0,0,0	0
7	O	G	2005	1/1	0.98	0.17	30,30,30,30	0
8	FES	B	201	4/4	0.98	0.03	9,10,10,10	0
4	MGD	G	2001	47/47	0.98	0.05	0,0,0,0	0
8	FES	F	201	4/4	0.98	0.03	7,7,7,7	0
4	MGD	G	2002	47/47	0.98	0.05	0,0,0,0	0
4	MGD	C	2001	47/47	0.98	0.06	0,0,0,0	0
6	F3S	C	2004	7/7	0.98	0.04	2,2,3,3	0
6	F3S	E	2004	7/7	0.98	0.03	0,0,0,0	0
4	MGD	A	2002	47/47	0.98	0.05	0,0,0,0	0
4	MGD	E	2001	47/47	0.98	0.06	0,0,0,0	0
4	MGD	E	2002	47/47	0.98	0.05	0,0,0,0	0
5	4MO	E	2003	1/1	0.99	0.02	0,0,0,0	0
6	F3S	G	2004	7/7	0.99	0.03	0,0,0,0	0
5	4MO	G	2003	1/1	0.99	0.02	1,1,1,1	0
5	4MO	A	2003	1/1	0.99	0.01	2,2,2,2	0
8	FES	H	201	4/4	0.99	0.03	5,5,5,6	0
5	4MO	C	2003	1/1	0.99	0.02	2,2,2,2	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

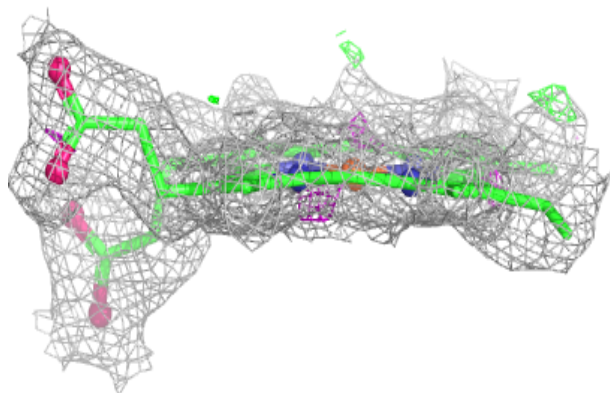
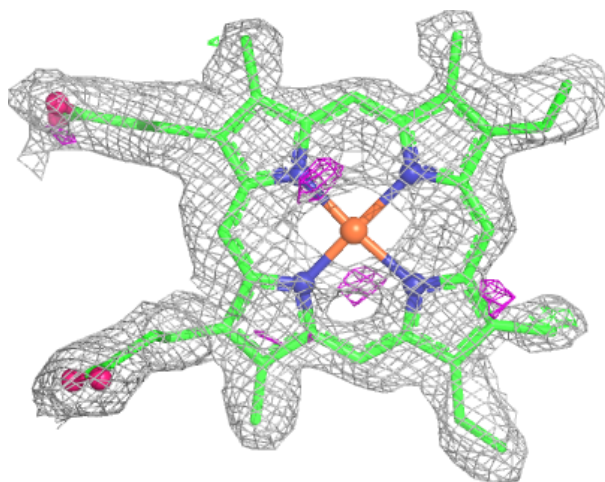
Electron density around HEM J 200:

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



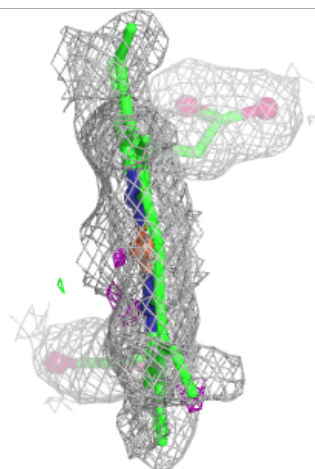
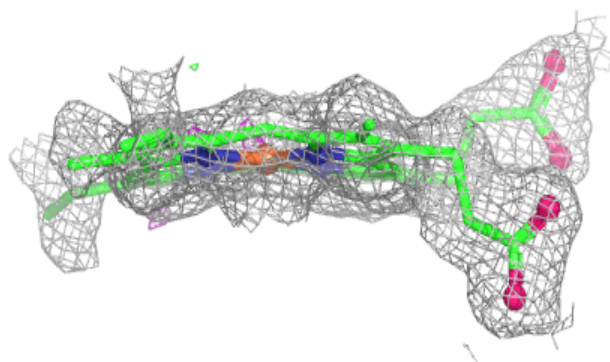
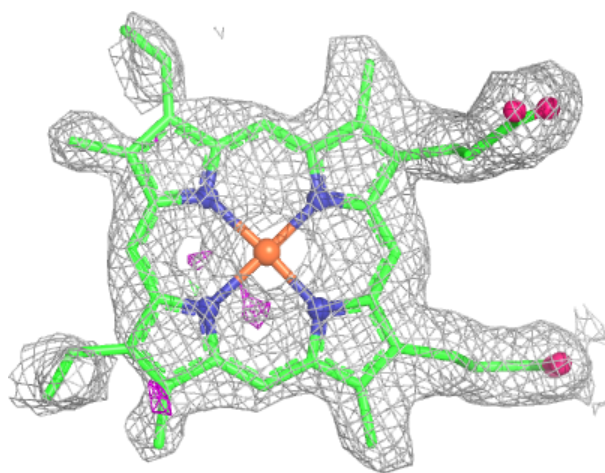
Electron density around HEM I 200:

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



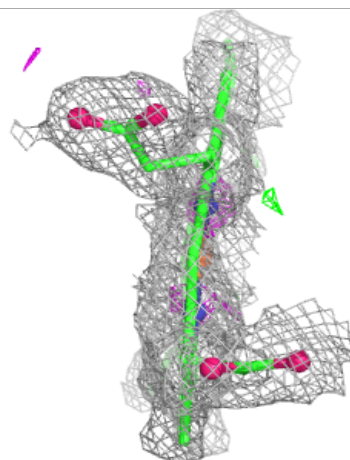
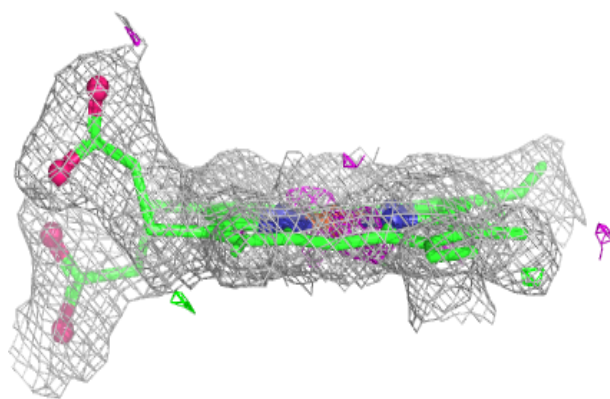
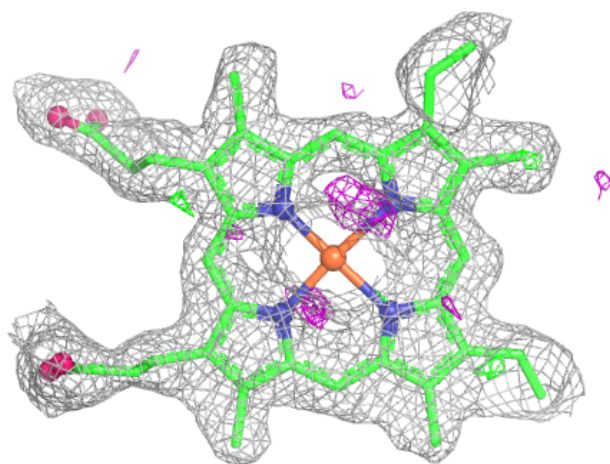
Electron density around HEM L 200:

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and green (positive)



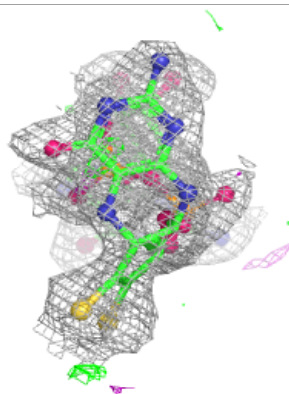
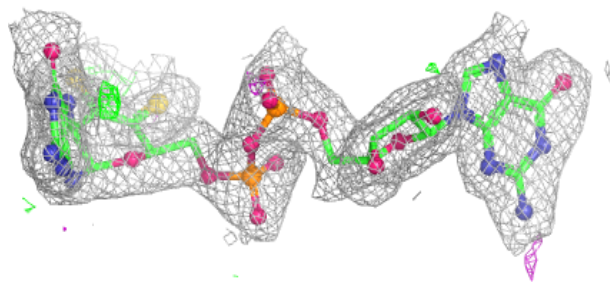
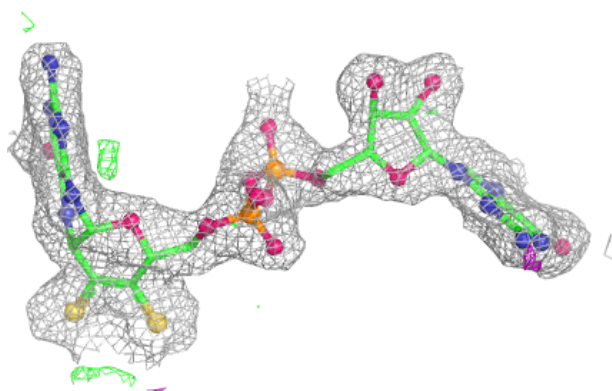
Electron density around HEC K 200:

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

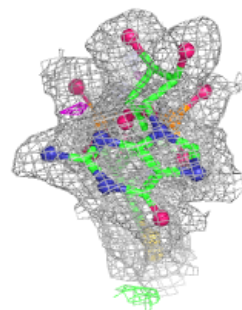
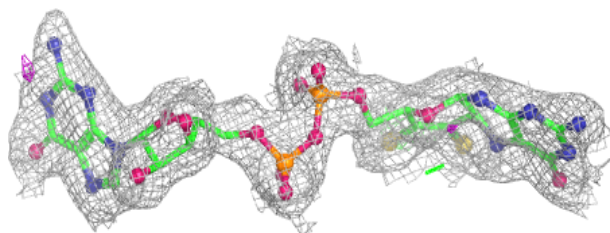
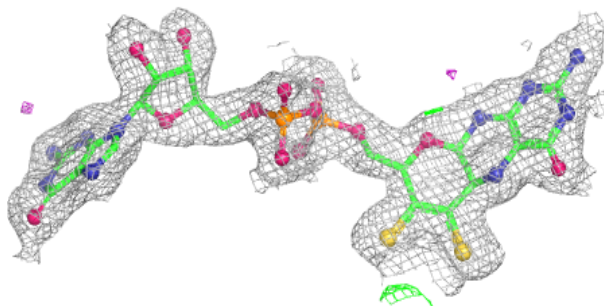


Electron density around MGD C 2002:

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

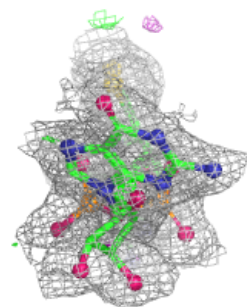
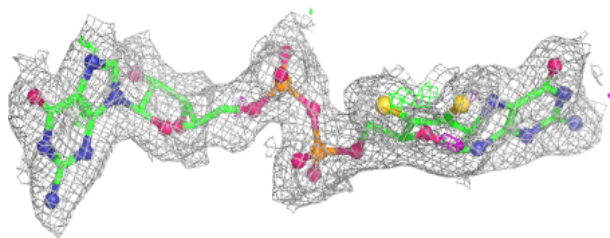
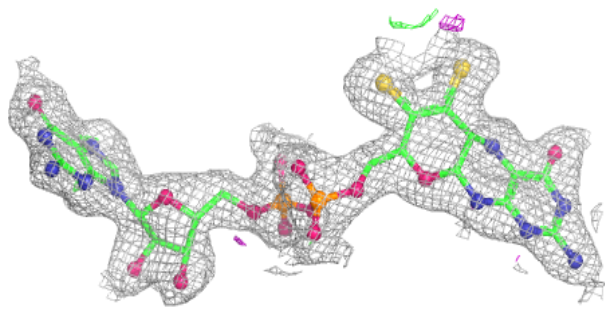
**Electron density around MGD A 2001:**

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

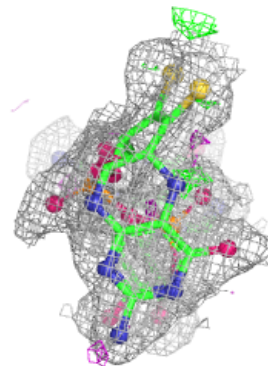
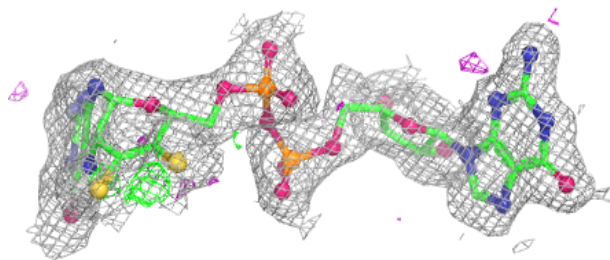
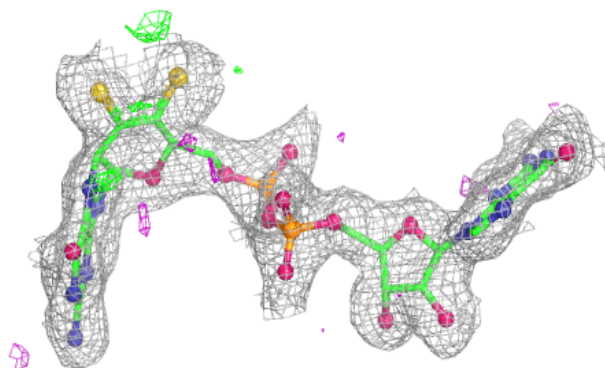


Electron density around MGD G 2001:

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

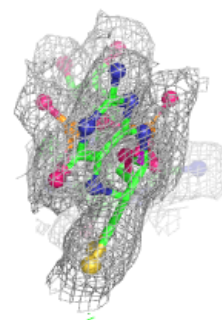
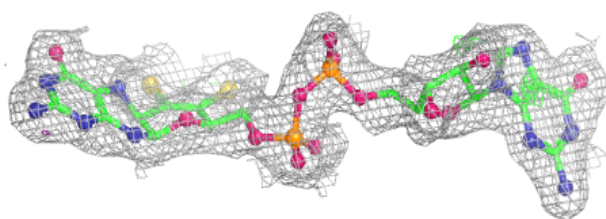
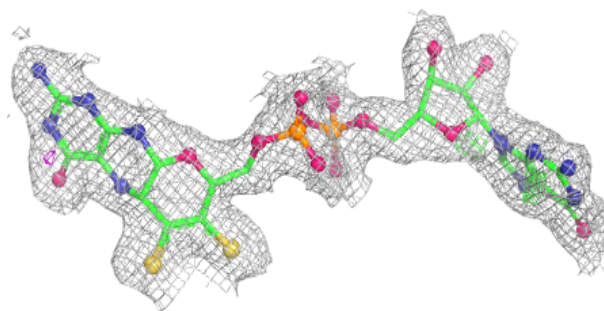
**Electron density around MGD G 2002:**

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

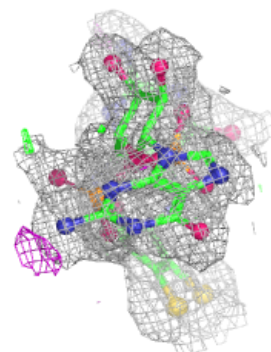
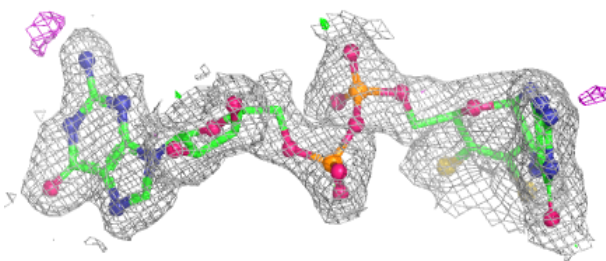
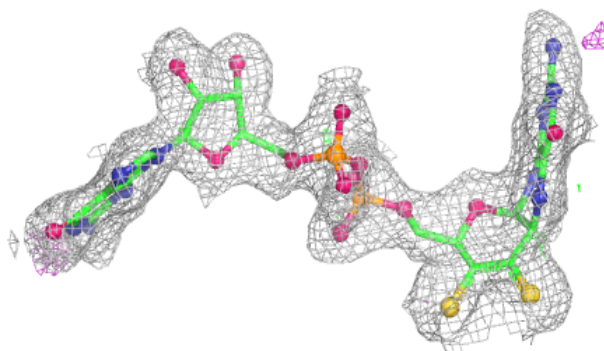


Electron density around MGD C 2001:

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

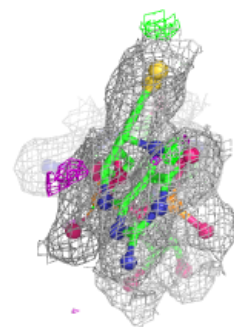
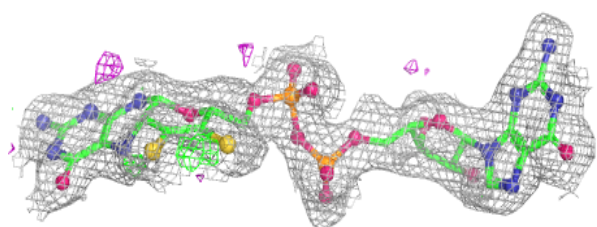
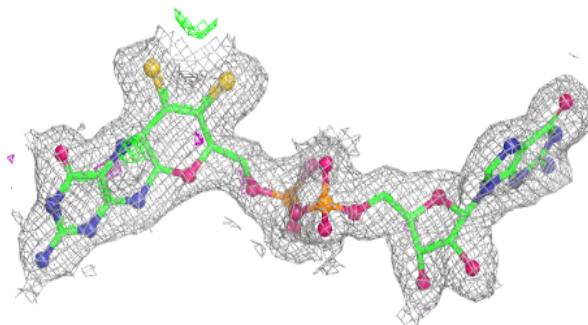
**Electron density around MGD A 2002:**

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

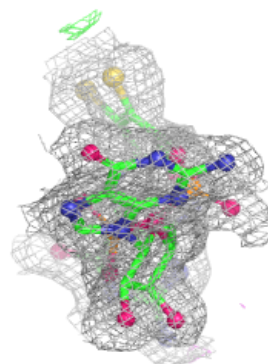
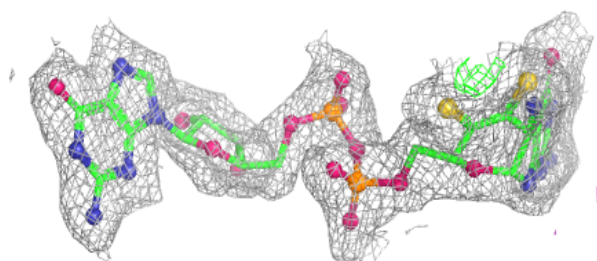
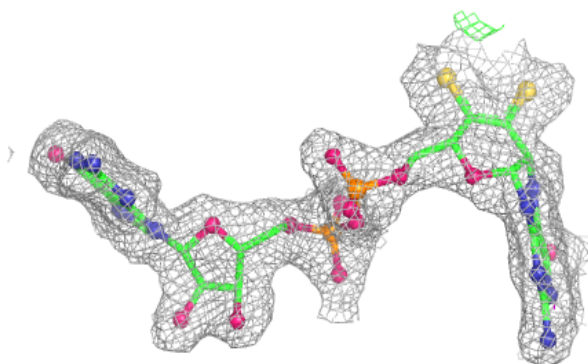


Electron density around MGD E 2001:

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

**Electron density around MGD E 2002:**

$2mF_o-DF_c$ (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.