



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 09:56 PM BST

PDB ID : 6E40
Title : Crystal structure of the indoleamine 2,3-dioxygenase 1 (IDO1) in complexed with ferric heme and Epacadostat
Authors : Luo, S.; Tong, L.
Deposited on : 2018-07-16
Resolution : 2.31 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

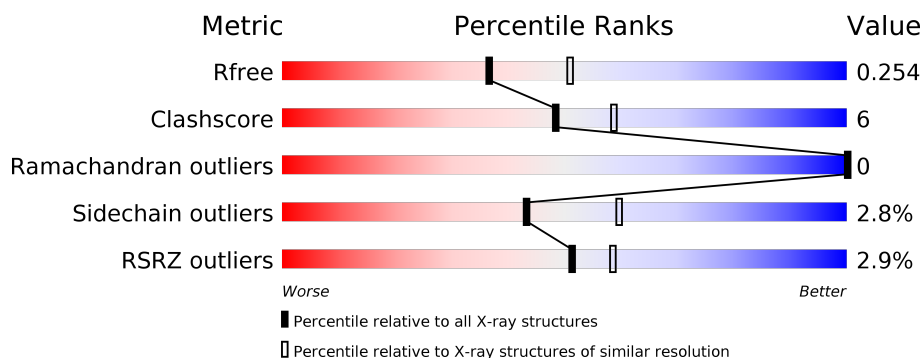
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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	405	<div> <div>0%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	405	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>9%</div> </div> </div>
1	C	405	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	405	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>7%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12155 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 Indoleamine 2,3-dioxygenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	0	0
			2924	1880	498	529	17			
1	B	369	Total	C	N	O	S	0	0	0
			2915	1875	497	526	17			
1	C	369	Total	C	N	O	S	0	0	0
			2915	1875	497	526	17			
1	D	378	Total	C	N	O	S	0	0	0
			2981	1915	509	540	17			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P14902
A	0	GLY	-	expression tag	UNP P14902
A	1	SER	-	expression tag	UNP P14902
A	2	SER	-	expression tag	UNP P14902
A	3	HIS	-	expression tag	UNP P14902
A	4	HIS	-	expression tag	UNP P14902
A	5	HIS	-	expression tag	UNP P14902
A	6	HIS	-	expression tag	UNP P14902
A	7	HIS	-	expression tag	UNP P14902
A	8	HIS	-	expression tag	UNP P14902
A	9	SER	-	expression tag	UNP P14902
A	10	SER	-	expression tag	UNP P14902
A	11	GLY	-	expression tag	UNP P14902
A	12	SER	-	expression tag	UNP P14902
A	13	ALA	-	expression tag	UNP P14902
A	14	ALA	-	expression tag	UNP P14902
A	116	ALA	LYS	engineered mutation	UNP P14902
A	117	ALA	LYS	engineered mutation	UNP P14902
B	-1	MET	-	initiating methionine	UNP P14902
B	0	GLY	-	expression tag	UNP P14902
B	1	SER	-	expression tag	UNP P14902

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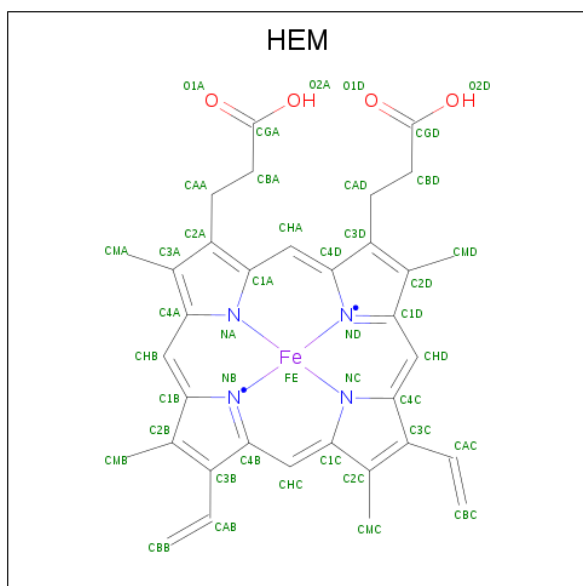
Chain	Residue	Modelled	Actual	Comment	Reference
B	2	SER	-	expression tag	UNP P14902
B	3	HIS	-	expression tag	UNP P14902
B	4	HIS	-	expression tag	UNP P14902
B	5	HIS	-	expression tag	UNP P14902
B	6	HIS	-	expression tag	UNP P14902
B	7	HIS	-	expression tag	UNP P14902
B	8	HIS	-	expression tag	UNP P14902
B	9	SER	-	expression tag	UNP P14902
B	10	SER	-	expression tag	UNP P14902
B	11	GLY	-	expression tag	UNP P14902
B	12	SER	-	expression tag	UNP P14902
B	13	ALA	-	expression tag	UNP P14902
B	14	ALA	-	expression tag	UNP P14902
B	116	ALA	LYS	engineered mutation	UNP P14902
B	117	ALA	LYS	engineered mutation	UNP P14902
C	-1	MET	-	initiating methionine	UNP P14902
C	0	GLY	-	expression tag	UNP P14902
C	1	SER	-	expression tag	UNP P14902
C	2	SER	-	expression tag	UNP P14902
C	3	HIS	-	expression tag	UNP P14902
C	4	HIS	-	expression tag	UNP P14902
C	5	HIS	-	expression tag	UNP P14902
C	6	HIS	-	expression tag	UNP P14902
C	7	HIS	-	expression tag	UNP P14902
C	8	HIS	-	expression tag	UNP P14902
C	9	SER	-	expression tag	UNP P14902
C	10	SER	-	expression tag	UNP P14902
C	11	GLY	-	expression tag	UNP P14902
C	12	SER	-	expression tag	UNP P14902
C	13	ALA	-	expression tag	UNP P14902
C	14	ALA	-	expression tag	UNP P14902
C	116	ALA	LYS	engineered mutation	UNP P14902
C	117	ALA	LYS	engineered mutation	UNP P14902
D	-1	MET	-	initiating methionine	UNP P14902
D	0	GLY	-	expression tag	UNP P14902
D	1	SER	-	expression tag	UNP P14902
D	2	SER	-	expression tag	UNP P14902
D	3	HIS	-	expression tag	UNP P14902
D	4	HIS	-	expression tag	UNP P14902
D	5	HIS	-	expression tag	UNP P14902
D	6	HIS	-	expression tag	UNP P14902
D	7	HIS	-	expression tag	UNP P14902

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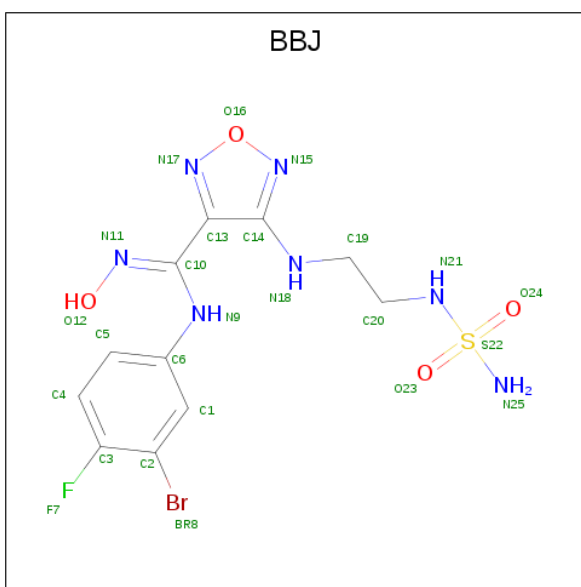
Chain	Residue	Modelled	Actual	Comment	Reference
D	8	HIS	-	expression tag	UNP P14902
D	9	SER	-	expression tag	UNP P14902
D	10	SER	-	expression tag	UNP P14902
D	11	GLY	-	expression tag	UNP P14902
D	12	SER	-	expression tag	UNP P14902
D	13	ALA	-	expression tag	UNP P14902
D	14	ALA	-	expression tag	UNP P14902
D	116	ALA	LYS	engineered mutation	UNP P14902
D	117	ALA	LYS	engineered mutation	UNP P14902

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
2	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
2	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

- Molecule 3 is N-(3-bromo-4-fluorophenyl)-N'-hydroxy-4-{[2-(sulfamoylamino)ethyl]amino}-1,2,5-oxadiazole-3-carboximidamide (three-letter code: BBJ) (formula: $C_{11}H_{13}BrFN_7O_4S$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	Br	C	F	N	O	S	0	0
			25	1	11	1	7	4	1		
3	B	1	Total	Br	C	F	N	O	S	0	0
			25	1	11	1	7	4	1		
3	D	1	Total	Br	C	F	N	O	S	0	0
			25	1	11	1	7	4	1		

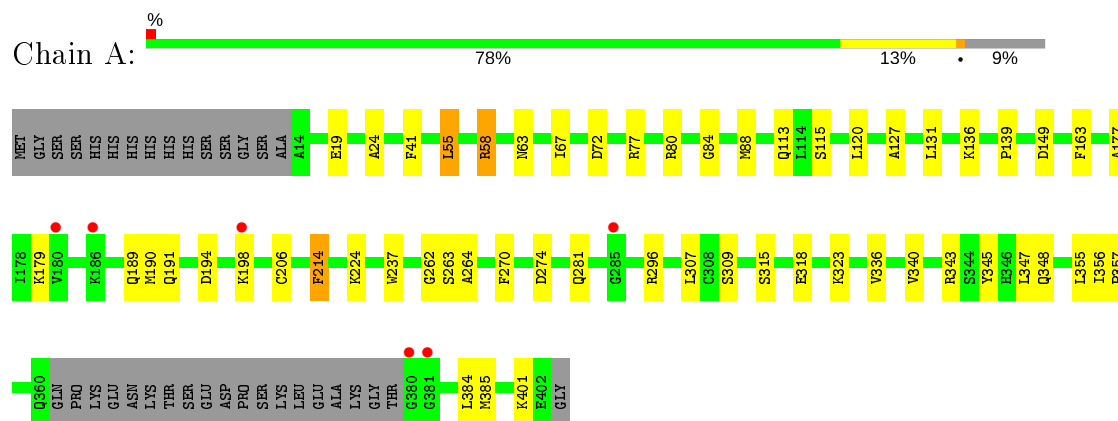
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	51	Total	O	0	0
			51	51		
4	B	41	Total	O	0	0
			41	41		
4	C	42	Total	O	0	0
			42	42		
4	D	39	Total	O	0	0
			39	39		

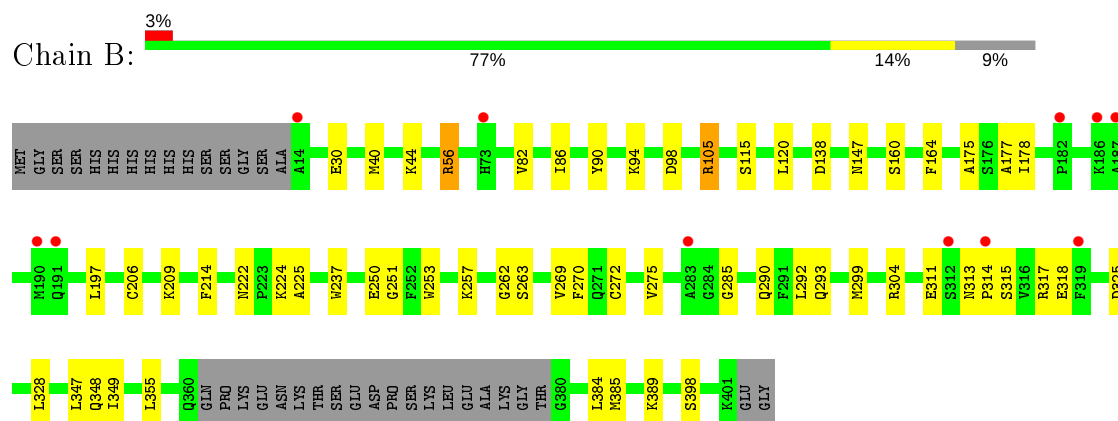
3 Residue-property plots

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

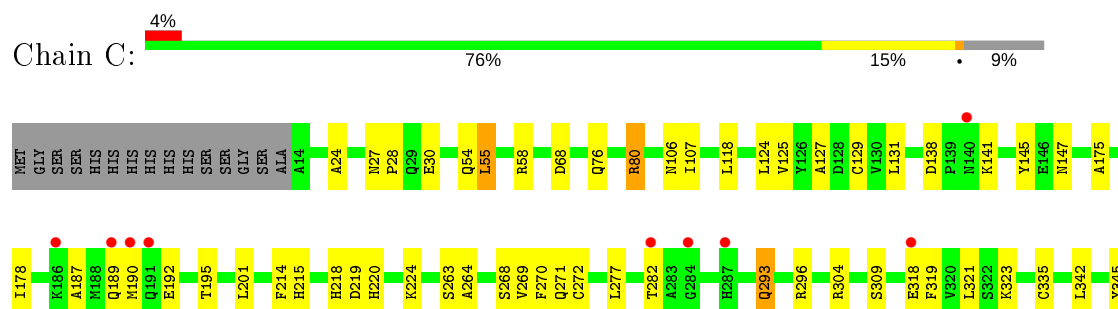
• Molecule 1: Indoleamine 2,3-dioxygenase 1



• Molecule 1: Indoleamine 2,3-dioxygenase 1

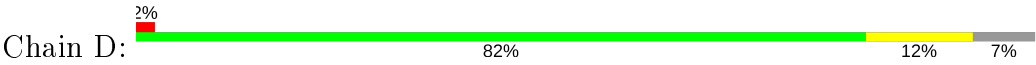


• Molecule 1: Indoleamine 2,3-dioxygenase 1





● Molecule 1: Indoleamine 2,3-dioxygenase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	80.37Å 200.14Å 114.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.86 – 2.31 46.86 – 2.31	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.86-2.31) 98.5 (46.86-2.31)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.12 _2829	Depositor
R, R_{free}	0.208 , 0.254 0.208 , 0.254	Depositor DCC
R_{free} test set	4029 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	49.8	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12155	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.90 % 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 1.6499e-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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.53	0/2992	0.64	3/4050 (0.1%)
1	B	0.70	0/2983	0.66	0/4038
1	C	0.66	0/2983	0.65	2/4038 (0.0%)
1	D	0.53	0/3049	0.64	0/4125
All	All	0.61	0/12007	0.65	5/16251 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	C	55	LEU	CA-CB-CG	-5.54	102.55	115.30
1	C	263	SER	C-N-CA	-5.39	108.22	121.70
1	A	55	LEU	CA-CB-CG	-5.12	103.53	115.30
1	A	58	ARG	NE-CZ-NH1	-5.08	117.76	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2924	0	2930	34	0
1	B	2915	0	2924	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2915	0	2924	43	0
1	D	2981	0	2995	26	0
2	A	43	0	30	5	0
2	B	43	0	30	5	0
2	C	43	0	30	2	0
2	D	43	0	30	3	0
3	A	25	0	0	3	0
3	B	25	0	0	3	0
3	D	25	0	0	0	0
4	A	51	0	0	3	0
4	B	41	0	0	0	0
4	C	42	0	0	3	0
4	D	39	0	0	1	0
All	All	12155	0	11893	143	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 (143) 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:C:215:HIS:HD2	1:C:345:TYR:CZ	1.74	1.05
1:A:296:ARG:HH21	1:A:307:LEU:HB3	1.22	1.02
1:C:219:ASP:OD1	4:C:601:HOH:O	1.78	1.00
1:C:215:HIS:CD2	1:C:345:TYR:CZ	2.60	0.90
1:C:282:THR:HG23	1:C:293:GLN:HE21	1.39	0.86
1:B:56:ARG:NH1	1:B:90:TYR:O	2.14	0.81
1:D:51:GLU:HG2	1:D:155:ARG:HH12	1.48	0.79
1:B:313:ASN:HB3	1:B:314:PRO:HD2	1.63	0.79
1:B:285:GLY:O	1:B:290:GLN:NE2	2.19	0.76
1:D:149:ASP:OD1	4:D:601:HOH:O	2.05	0.73
1:C:282:THR:CG2	1:C:293:GLN:HE21	2.02	0.72
1:B:138:ASP:H	1:B:147:ASN:HD21	1.39	0.70
1:B:317:ARG:NH1	1:B:398:SER:O	2.24	0.69
1:D:175:ALA:HA	1:D:178:ILE:HD12	1.75	0.69
1:D:115:SER:HB3	1:D:120:LEU:O	1.93	0.68
1:B:105:ARG:HG2	1:B:250:GLU:HG2	1.76	0.68
1:C:224:LYS:H	1:C:224:LYS:HD2	1.58	0.67
1:B:299:MET:O	1:B:304:ARG:NH1	2.29	0.66
1:A:347:LEU:HD22	4:A:608:HOH:O	1.96	0.64
1:C:271:GLN:OE1	1:C:296:ARG:HD3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:PHE:CD2	2:A:501:HEM:HMD3	2.33	0.63
1:A:315:SER:HB3	1:A:318:GLU:HB2	1.80	0.62
1:C:282:THR:HG23	1:C:293:GLN:NE2	2.14	0.62
1:A:296:ARG:NH2	1:A:307:LEU:HB3	2.05	0.61
2:A:501:HEM:HBB2	2:A:501:HEM:HMB1	1.82	0.60
1:B:115:SER:HB3	1:B:120:LEU:O	2.01	0.60
1:A:41:PHE:HE2	1:A:58:ARG:HH12	1.51	0.59
1:C:264:ALA:HB3	2:C:501:HEM:C4C	2.39	0.58
1:C:215:HIS:HD2	1:C:345:TYR:OH	1.85	0.58
1:B:56:ARG:NH2	1:B:98:ASP:O	2.31	0.57
1:D:51:GLU:HG2	1:D:155:ARG:NH1	2.17	0.56
1:D:227:PHE:O	1:D:231:ARG:NH1	2.34	0.56
1:B:175:ALA:HA	1:B:178:ILE:HD12	1.87	0.56
1:D:127:ALA:HA	1:D:131:LEU:HG	1.87	0.55
1:A:72:ASP:OD1	1:A:72:ASP:N	2.40	0.55
1:B:315:SER:HB3	1:B:318:GLU:HG3	1.89	0.55
1:C:138:ASP:OD2	1:C:141:LYS:HG3	2.07	0.54
1:C:127:ALA:HA	1:C:131:LEU:HD12	1.88	0.54
1:A:194:ASP:O	1:A:198:LYS:HG2	2.08	0.53
1:B:253:TRP:CE3	1:B:257:LYS:HD3	2.43	0.53
1:A:264:ALA:HB3	2:A:501:HEM:C4C	2.45	0.52
1:C:215:HIS:CD2	1:C:345:TYR:CE1	2.98	0.51
1:D:51:GLU:O	1:D:94:LYS:NZ	2.43	0.51
1:D:177:ALA:HB2	1:D:206:CYS:HB2	1.93	0.51
1:C:145:TYR:CZ	1:C:220:HIS:CE1	2.98	0.51
1:A:84:GLY:O	1:A:88:MET:HG2	2.11	0.51
1:B:313:ASN:CB	1:B:314:PRO:HD2	2.38	0.51
1:B:275:VAL:HG13	1:B:311:GLU:HG3	1.93	0.50
1:D:275:VAL:CG1	1:D:311:GLU:HG2	2.42	0.50
1:A:343:ARG:O	1:A:347:LEU:HD23	2.12	0.50
1:D:23:PHE:HD2	1:D:269:VAL:HG23	1.76	0.50
1:A:262:GLY:HA3	3:A:502:BBJ:BR8	2.67	0.49
1:C:27:ASN:N	1:C:28:PRO:HD3	2.27	0.49
1:A:19:GLU:HG3	1:A:179:LYS:HD3	1.94	0.49
1:B:40:MET:HE2	1:B:44:LYS:HD2	1.93	0.49
1:A:127:ALA:HA	1:A:131:LEU:HD12	1.93	0.49
1:C:106:ASN:HB2	4:C:608:HOH:O	2.11	0.48
1:B:138:ASP:N	1:B:147:ASN:HD21	2.08	0.48
2:B:501:HEM:HBB2	2:B:501:HEM:HMB1	1.95	0.48
2:A:501:HEM:CMB	2:A:501:HEM:HBB2	2.44	0.48
1:C:54:GLN:O	1:C:58:ARG:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:375:GLU:O	1:D:381:GLY:HA3	2.13	0.48
1:A:136:LYS:HD3	1:A:139:PRO:HA	1.95	0.48
1:C:187:ALA:HB2	1:C:195:THR:HG22	1.96	0.48
1:B:347:LEU:HD22	1:B:385:MET:SD	2.54	0.48
1:A:191:GLN:OE1	1:A:323:LYS:NZ	2.47	0.47
1:D:333:ASP:O	1:D:337:LYS:HG3	2.14	0.47
1:B:313:ASN:HB3	1:B:314:PRO:CD	2.36	0.47
1:C:55:LEU:HG	1:C:55:LEU:O	2.07	0.47
1:D:135:LYS:HB2	1:D:135:LYS:HE3	1.71	0.47
1:B:292:LEU:HD23	1:B:292:LEU:HA	1.79	0.47
1:C:318:GLU:HA	1:C:321:LEU:HD12	1.96	0.47
1:D:317:ARG:NH1	1:D:398:SER:O	2.33	0.47
1:B:197:LEU:HD23	1:B:328:LEU:HD23	1.97	0.47
1:C:175:ALA:HA	1:C:178:ILE:HD12	1.96	0.47
1:D:72:ASP:O	1:D:76:GLN:HG3	2.14	0.47
1:A:189:GLN:OE1	1:D:189:GLN:NE2	2.46	0.46
1:B:177:ALA:HB2	1:B:206:CYS:HB2	1.97	0.46
1:C:346:HIS:HE1	2:C:501:HEM:NA	2.08	0.46
1:C:145:TYR:CZ	1:C:220:HIS:ND1	2.84	0.46
1:C:269:VAL:HG12	1:C:270:PHE:HD1	1.81	0.46
1:D:275:VAL:HG13	1:D:311:GLU:HG2	1.97	0.46
1:A:355:LEU:HD11	1:A:385:MET:HG3	1.97	0.45
1:D:160:SER:HB2	1:D:164:PHE:CE2	2.52	0.45
1:A:67:ILE:HG12	4:A:601:HOH:O	2.15	0.45
1:A:163:PHE:CZ	3:A:502:BBJ:C5	3.00	0.45
2:B:501:HEM:C4A	3:B:502:BBJ:N11	2.85	0.45
1:C:215:HIS:CD2	1:C:345:TYR:OH	2.68	0.44
1:D:339:LEU:HA	1:D:339:LEU:HD23	1.86	0.44
1:C:277:LEU:HD11	1:C:335:CYS:HB3	1.99	0.44
1:A:274:ASP:OD2	1:A:281:GLN:HG3	2.17	0.44
2:B:501:HEM:NA	3:B:502:BBJ:N11	2.66	0.44
1:B:105:ARG:HD2	1:B:251:GLY:HA3	2.00	0.44
1:C:189:GLN:HG2	1:C:190:MET:CE	2.48	0.43
1:B:269:VAL:HG12	1:B:270:PHE:HD1	1.82	0.43
1:C:192:GLU:HG2	1:C:195:THR:HB	2.00	0.43
1:A:384:LEU:HD11	2:A:501:HEM:HMA3	2.01	0.43
1:C:107:ILE:HD13	1:C:107:ILE:HG21	1.78	0.43
1:D:179:LYS:O	1:D:182:PRO:HD2	2.19	0.43
1:B:222:ASN:HD22	1:B:225:ALA:HB2	1.84	0.43
1:C:224:LYS:N	1:C:224:LYS:HD2	2.31	0.43
1:B:385:MET:HG3	1:B:389:LYS:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ARG:HD2	1:A:77:ARG:HA	1.87	0.43
1:C:145:TYR:CE1	1:C:220:HIS:CE1	3.07	0.43
1:A:214:PHE:HD1	1:A:214:PHE:O	2.02	0.42
1:A:336:VAL:O	1:A:340:VAL:HG23	2.19	0.42
1:B:355:LEU:HD11	1:B:385:MET:CE	2.49	0.42
1:A:345:TYR:O	1:A:348:GLN:HB2	2.20	0.42
1:B:160:SER:HB2	1:B:164:PHE:CE2	2.54	0.42
1:B:262:GLY:HA3	3:B:502:BBJ:BR8	2.75	0.42
1:A:177:ALA:HB2	1:A:206:CYS:HB2	2.01	0.42
1:A:189:GLN:HE21	1:A:190:MET:CE	2.33	0.42
1:B:384:LEU:HD11	2:B:501:HEM:HMA3	2.01	0.42
1:A:356:ILE:HB	1:A:357:PRO:HD3	2.02	0.42
1:B:270:PHE:CD2	2:B:501:HEM:HMD3	2.55	0.42
1:C:356:ILE:HB	1:C:357:PRO:HD3	2.01	0.42
1:B:82:VAL:O	1:B:86:ILE:HG13	2.20	0.42
1:C:296:ARG:O	1:C:304:ARG:HD3	2.20	0.42
1:D:54:GLN:HE21	1:D:58:ARG:NH2	2.18	0.41
1:D:397:LYS:HB3	1:D:397:LYS:HE3	1.85	0.41
2:D:501:HEM:HMB1	2:D:501:HEM:HBB2	2.01	0.41
1:A:263:SER:HA	3:A:502:BBJ:C10	2.50	0.41
1:C:319:PHE:O	1:C:323:LYS:HG2	2.20	0.41
1:A:24:ALA:HA	1:A:131:LEU:HB3	2.02	0.41
1:A:115:SER:HB3	1:A:120:LEU:O	2.19	0.41
1:C:270:PHE:CZ	1:C:342:LEU:HB3	2.55	0.41
1:A:113:GLN:OE1	4:A:601:HOH:O	2.22	0.41
1:C:124:LEU:HD21	1:C:129:CYS:HB3	2.03	0.41
1:C:268:SER:O	1:C:272:CYS:HB2	2.20	0.41
4:C:639:HOH:O	1:D:67:ILE:HD11	2.19	0.41
1:B:325:ASP:HB3	1:B:328:LEU:HB2	2.03	0.41
1:C:24:ALA:HA	1:C:131:LEU:HB3	2.02	0.41
1:B:315:SER:HB3	1:B:318:GLU:CG	2.51	0.41
1:A:189:GLN:HG2	1:A:190:MET:HE2	2.03	0.41
1:C:76:GLN:HB3	1:C:118:LEU:HD11	2.03	0.41
2:D:501:HEM:HHA	2:D:501:HEM:HBA2	2.03	0.41
1:C:138:ASP:N	1:C:147:ASN:OD1	2.52	0.40
1:C:218:HIS:CE1	1:C:352:LYS:HD2	2.56	0.40
1:B:349:ILE:HA	1:B:349:ILE:HD13	1.88	0.40
1:C:201:LEU:HA	1:C:201:LEU:HD23	1.95	0.40
1:D:264:ALA:HB3	2:D:501:HEM:C4C	2.56	0.40
1:D:325:ASP:HB3	1:D:328:LEU:HB2	2.04	0.40
1:C:80:ARG:HH21	1:C:125:VAL:HG22	1.87	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	366/405 (90%)	357 (98%)	9 (2%)	0	100	100
1	B	365/405 (90%)	352 (96%)	13 (4%)	0	100	100
1	C	365/405 (90%)	350 (96%)	15 (4%)	0	100	100
1	D	374/405 (92%)	361 (96%)	13 (4%)	0	100	100
All	All	1470/1620 (91%)	1420 (97%)	50 (3%)	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	317/346 (92%)	309 (98%)	8 (2%)	47	65
1	B	316/346 (91%)	304 (96%)	12 (4%)	33	47
1	C	316/346 (91%)	308 (98%)	8 (2%)	47	65
1	D	323/346 (93%)	316 (98%)	7 (2%)	52	69
All	All	1272/1384 (92%)	1237 (97%)	35 (3%)	43	60

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LEU
1	A	63	ASN
1	A	149	ASP
1	A	214	PHE
1	A	224	LYS
1	A	237	TRP
1	A	309	SER
1	A	401	LYS
1	B	30	GLU
1	B	56	ARG
1	B	94	LYS
1	B	105	ARG
1	B	209	LYS
1	B	214	PHE
1	B	224	LYS
1	B	237	TRP
1	B	263	SER
1	B	272	CYS
1	B	293	GLN
1	B	348	GLN
1	C	30	GLU
1	C	68	ASP
1	C	80	ARG
1	C	214	PHE
1	C	293	GLN
1	C	309	SER
1	C	383	ASP
1	C	384	LEU
1	D	57	GLU
1	D	214	PHE
1	D	237	TRP
1	D	263	SER
1	D	272	CYS
1	D	287	HIS
1	D	372	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	147	ASN
1	B	222	ASN
1	B	290	GLN
1	C	189	GLN

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Mol	Chain	Res	Type
1	C	215	HIS
1	C	218	HIS
1	C	290	GLN
1	C	293	GLN
1	C	348	GLN
1	C	360	GLN
1	D	293	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	D	501	1,3	27,50,50	1.97	5 (18%)	17,82,82	1.57	3 (17%)
3	BBJ	D	502	2	21,26,26	2.53	5 (23%)	23,36,36	2.19	5 (21%)
3	BBJ	B	502	2	21,26,26	2.82	5 (23%)	23,36,36	2.19	5 (21%)
2	HEM	B	501	1,3	27,50,50	1.95	6 (22%)	17,82,82	2.04	7 (41%)
2	HEM	C	501	1	27,50,50	1.80	5 (18%)	17,82,82	2.03	10 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BBJ	A	502	2	21,26,26	2.69	4 (19%)	23,36,36	2.20	5 (21%)
2	HEM	A	501	1,3	27,50,50	1.85	4 (14%)	17,82,82	1.95	8 (47%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	D	501	1,3	-	0/6/54/54	-
3	BBJ	D	502	2	-	3/11/18/18	0/2/2/2
3	BBJ	B	502	2	-	1/11/18/18	0/2/2/2
2	HEM	B	501	1,3	-	1/6/54/54	-
2	HEM	C	501	1	-	1/6/54/54	-
3	BBJ	A	502	2	-	1/11/18/18	0/2/2/2
2	HEM	A	501	1,3	-	1/6/54/54	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	BBJ	C14-N18	7.92	1.46	1.34
3	A	502	BBJ	C14-N18	7.81	1.46	1.34
3	B	502	BBJ	C13-C10	7.62	1.57	1.47
3	D	502	BBJ	C14-N18	7.32	1.46	1.34
3	A	502	BBJ	C13-C10	6.96	1.56	1.47
3	D	502	BBJ	C13-C10	5.89	1.55	1.47
2	B	501	HEM	C3C-C2C	-5.15	1.33	1.40
3	A	502	BBJ	C10-N9	4.94	1.46	1.36
3	B	502	BBJ	C10-N9	4.93	1.46	1.36
3	D	502	BBJ	C10-N9	4.85	1.45	1.36
2	D	501	HEM	C3C-C2C	-4.78	1.33	1.40
2	A	501	HEM	C3C-C2C	-4.40	1.34	1.40
2	D	501	HEM	C3B-CAB	4.28	1.56	1.47
2	B	501	HEM	C3B-C2B	-4.13	1.34	1.40
2	D	501	HEM	C3B-C2B	-3.90	1.35	1.40
2	C	501	HEM	C3C-CAC	3.84	1.55	1.47
2	A	501	HEM	C3B-CAB	3.84	1.55	1.47
2	C	501	HEM	C3B-CAB	3.81	1.55	1.47
2	A	501	HEM	C3B-C2B	-3.78	1.35	1.40
2	C	501	HEM	C3C-C2C	-3.76	1.35	1.40
2	B	501	HEM	C3B-CAB	3.57	1.55	1.47
2	D	501	HEM	C3C-CAC	3.46	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3C-CAC	3.43	1.54	1.47
2	C	501	HEM	C3B-C2B	-3.41	1.35	1.40
2	B	501	HEM	C3C-CAC	3.28	1.54	1.47
3	D	502	BBJ	BR8-C2	3.06	1.96	1.89
3	B	502	BBJ	S22-N21	2.76	1.73	1.62
3	B	502	BBJ	BR8-C2	2.70	1.96	1.89
2	B	501	HEM	CAA-C2A	2.63	1.55	1.52
2	D	501	HEM	CAA-C2A	2.61	1.55	1.52
3	D	502	BBJ	S22-N21	2.44	1.71	1.62
3	A	502	BBJ	S22-N21	2.43	1.71	1.62
2	B	501	HEM	CMC-C2C	2.11	1.56	1.51
2	C	501	HEM	CAA-C2A	2.00	1.55	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	BBJ	O24-S22-O23	-8.27	101.02	119.96
3	B	502	BBJ	O24-S22-O23	-8.16	101.29	119.96
3	D	502	BBJ	O24-S22-O23	-8.06	101.51	119.96
2	B	501	HEM	CMA-C3A-C4A	-3.78	122.65	128.46
2	B	501	HEM	C4A-C3A-C2A	3.68	109.55	107.00
2	A	501	HEM	C1D-C2D-C3D	3.53	109.45	107.00
2	A	501	HEM	C4C-C3C-C2C	3.52	109.35	106.90
3	D	502	BBJ	N9-C10-N11	-3.27	118.74	123.68
3	B	502	BBJ	N9-C10-N11	-3.26	118.76	123.68
2	D	501	HEM	CAA-CBA-CGA	-3.26	107.20	112.67
3	A	502	BBJ	N9-C10-N11	-3.24	118.80	123.68
2	C	501	HEM	C1D-C2D-C3D	3.20	109.22	107.00
2	C	501	HEM	CMB-C2B-C3B	3.16	130.59	124.68
3	D	502	BBJ	C6-N9-C10	-3.12	121.74	128.25
3	B	502	BBJ	C6-N9-C10	-2.91	122.17	128.25
3	A	502	BBJ	C6-N9-C10	-2.83	122.35	128.25
2	C	501	HEM	CBA-CAA-C2A	-2.80	107.33	112.49
2	A	501	HEM	CMB-C2B-C3B	2.58	129.50	124.68
2	B	501	HEM	C4C-C3C-C2C	2.57	108.70	106.90
2	B	501	HEM	C1D-C2D-C3D	2.50	108.74	107.00
2	D	501	HEM	CMA-C3A-C4A	-2.49	124.64	128.46
2	B	501	HEM	CAA-CBA-CGA	-2.48	108.51	112.67
2	C	501	HEM	CAD-CBD-CGD	-2.48	108.51	112.67
2	C	501	HEM	C4C-C3C-C2C	2.47	108.62	106.90
2	D	501	HEM	C4A-C3A-C2A	2.41	108.67	107.00
2	A	501	HEM	CBD-CAD-C3D	-2.37	108.11	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	CMB-C2B-C3B	2.33	129.04	124.68
2	C	501	HEM	CMD-C2D-C1D	-2.33	124.89	128.46
3	B	502	BBJ	O24-S22-N21	2.32	111.44	106.88
3	A	502	BBJ	O24-S22-N21	2.26	111.32	106.88
3	A	502	BBJ	O23-S22-N21	2.25	111.29	106.88
3	D	502	BBJ	O23-S22-N21	2.24	111.29	106.88
2	A	501	HEM	CBA-CAA-C2A	-2.23	108.38	112.49
2	A	501	HEM	C4A-C3A-C2A	2.20	108.53	107.00
2	A	501	HEM	CMA-C3A-C4A	-2.19	125.10	128.46
3	B	502	BBJ	O23-S22-N21	2.18	111.16	106.88
3	D	502	BBJ	O24-S22-N21	2.16	111.12	106.88
2	B	501	HEM	CBA-CAA-C2A	-2.16	108.51	112.49
2	C	501	HEM	CBD-CAD-C3D	-2.10	108.60	112.48
2	A	501	HEM	C3C-C4C-NC	-2.09	107.01	110.94
2	C	501	HEM	CMA-C3A-C4A	-2.08	125.26	128.46
2	C	501	HEM	C3C-C4C-NC	-2.07	107.03	110.94
2	C	501	HEM	C4A-C3A-C2A	2.03	108.41	107.00

There are no chirality outliers.

All (8) torsion outliers are listed below:

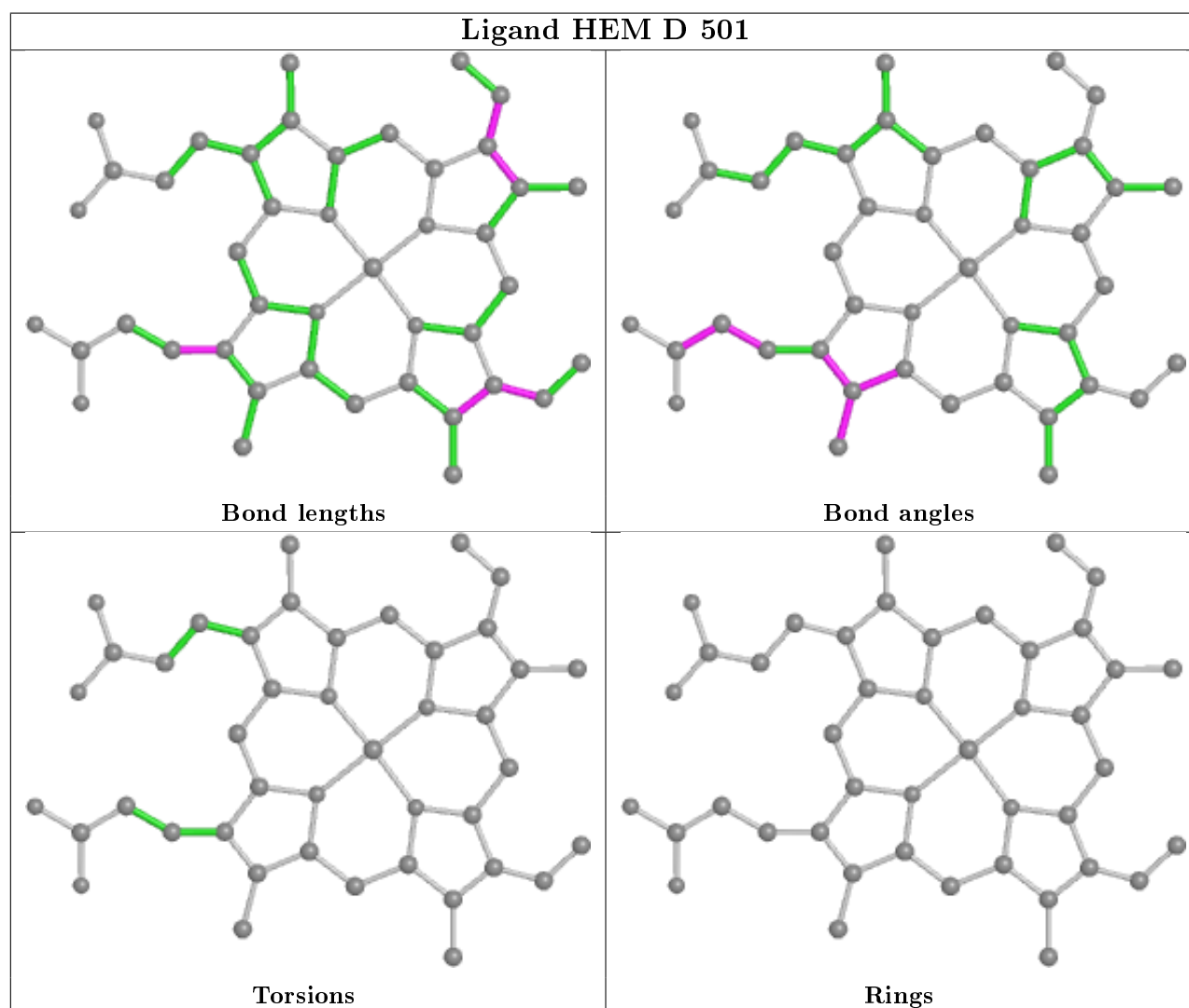
Mol	Chain	Res	Type	Atoms
3	D	502	BBJ	C20-N21-S22-O24
2	B	501	HEM	C2A-CAA-CBA-CGA
2	C	501	HEM	C2A-CAA-CBA-CGA
2	A	501	HEM	C2A-CAA-CBA-CGA
3	A	502	BBJ	N18-C19-C20-N21
3	B	502	BBJ	N18-C19-C20-N21
3	D	502	BBJ	N18-C19-C20-N21
3	D	502	BBJ	C20-N21-S22-O23

There are no ring outliers.

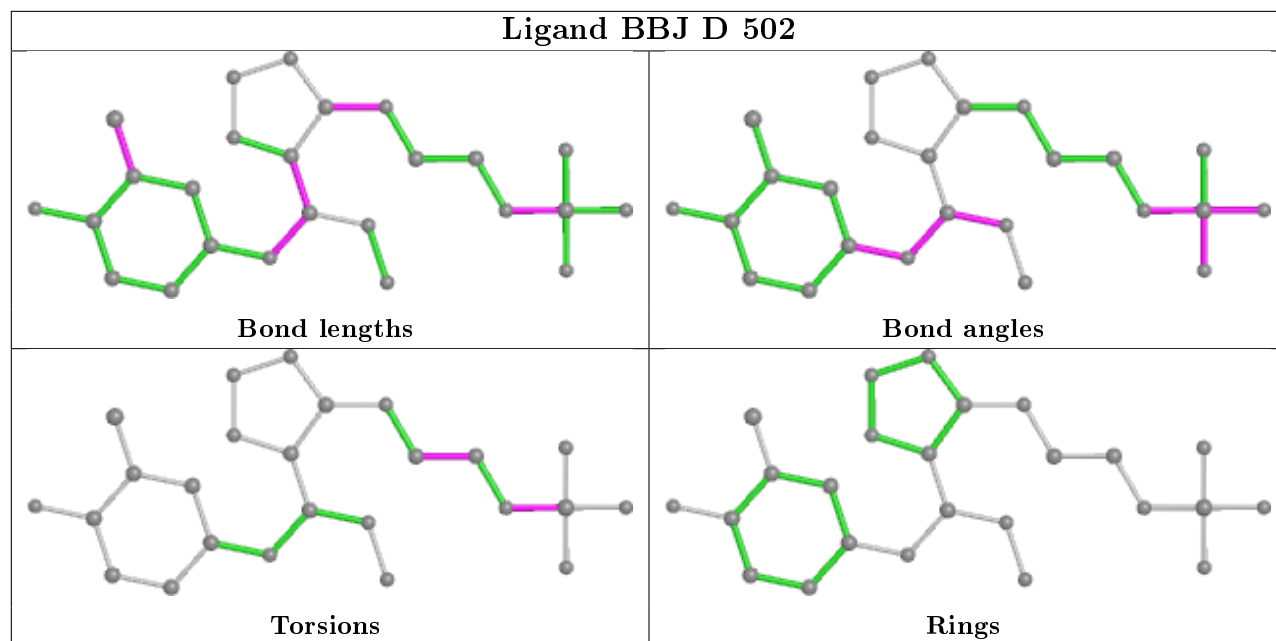
6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	HEM	3	0
3	B	502	BBJ	3	0
2	B	501	HEM	5	0
2	C	501	HEM	2	0
3	A	502	BBJ	3	0
2	A	501	HEM	5	0

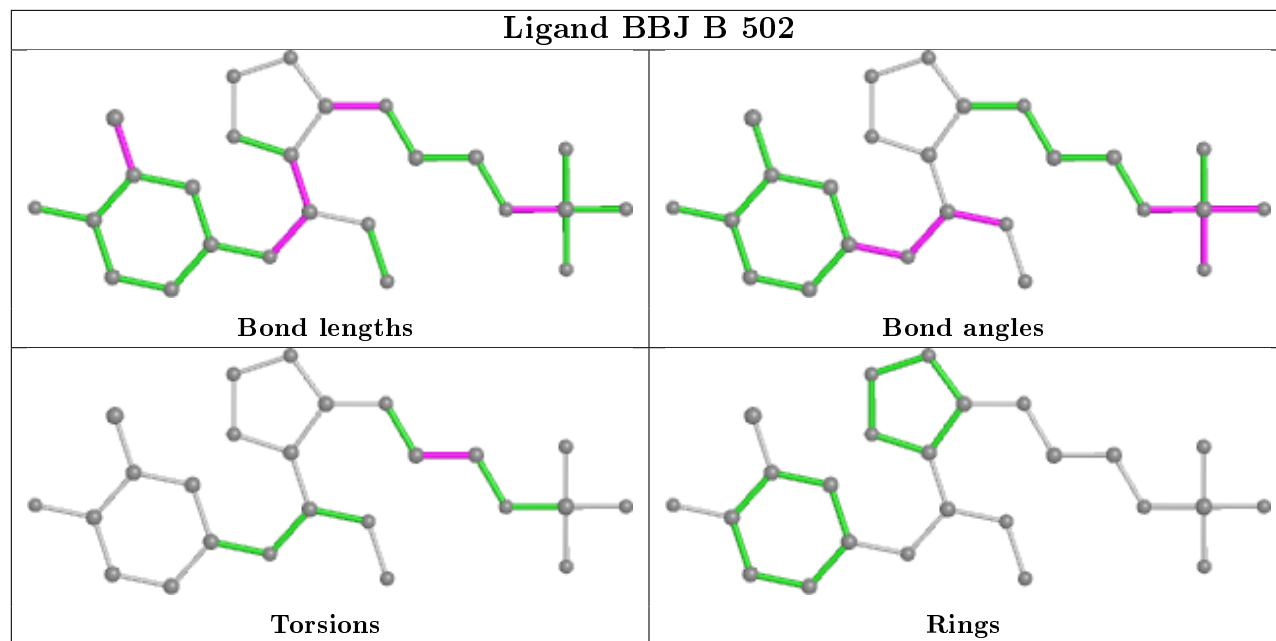
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

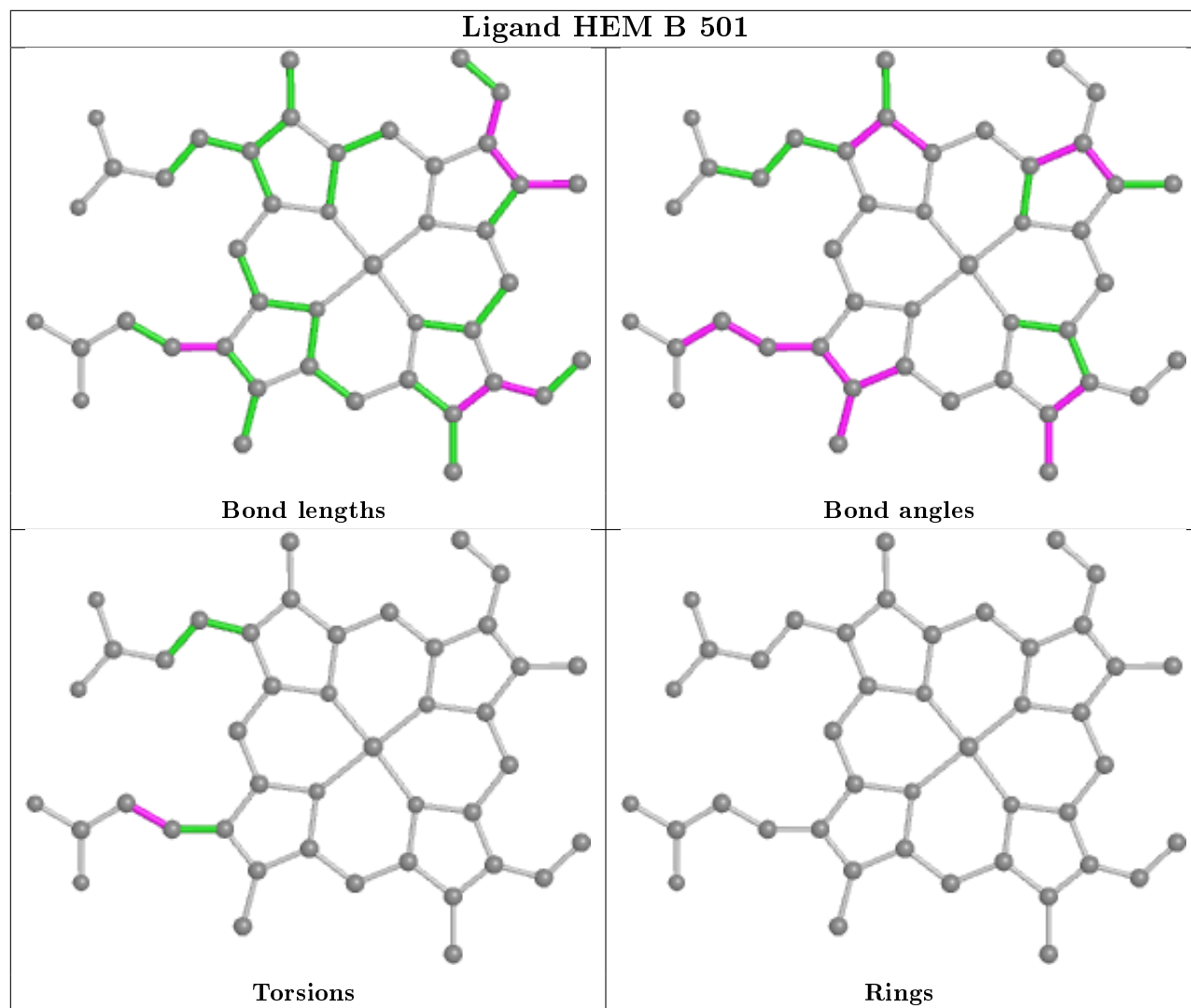


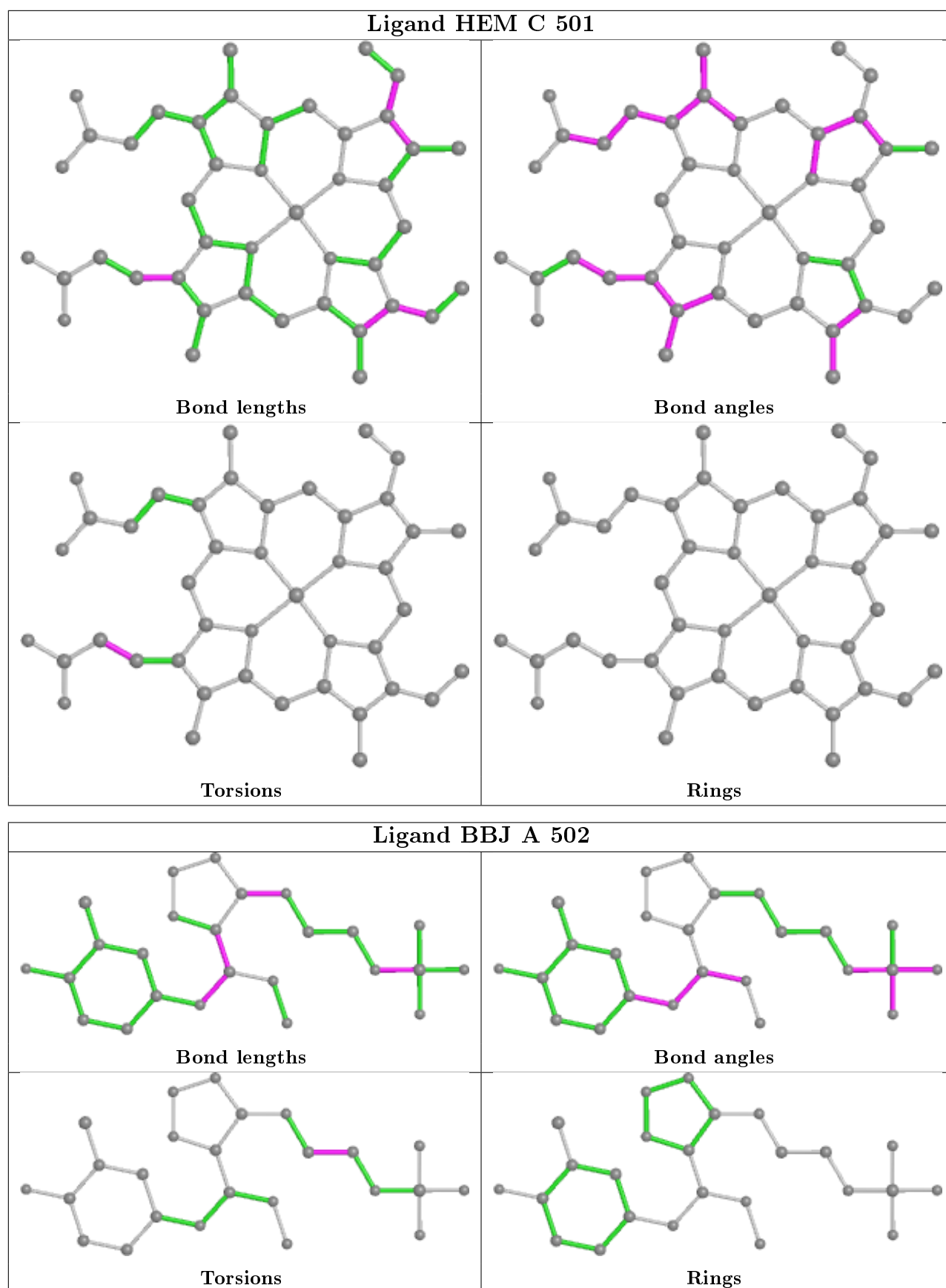
Ligand BBJ D 502

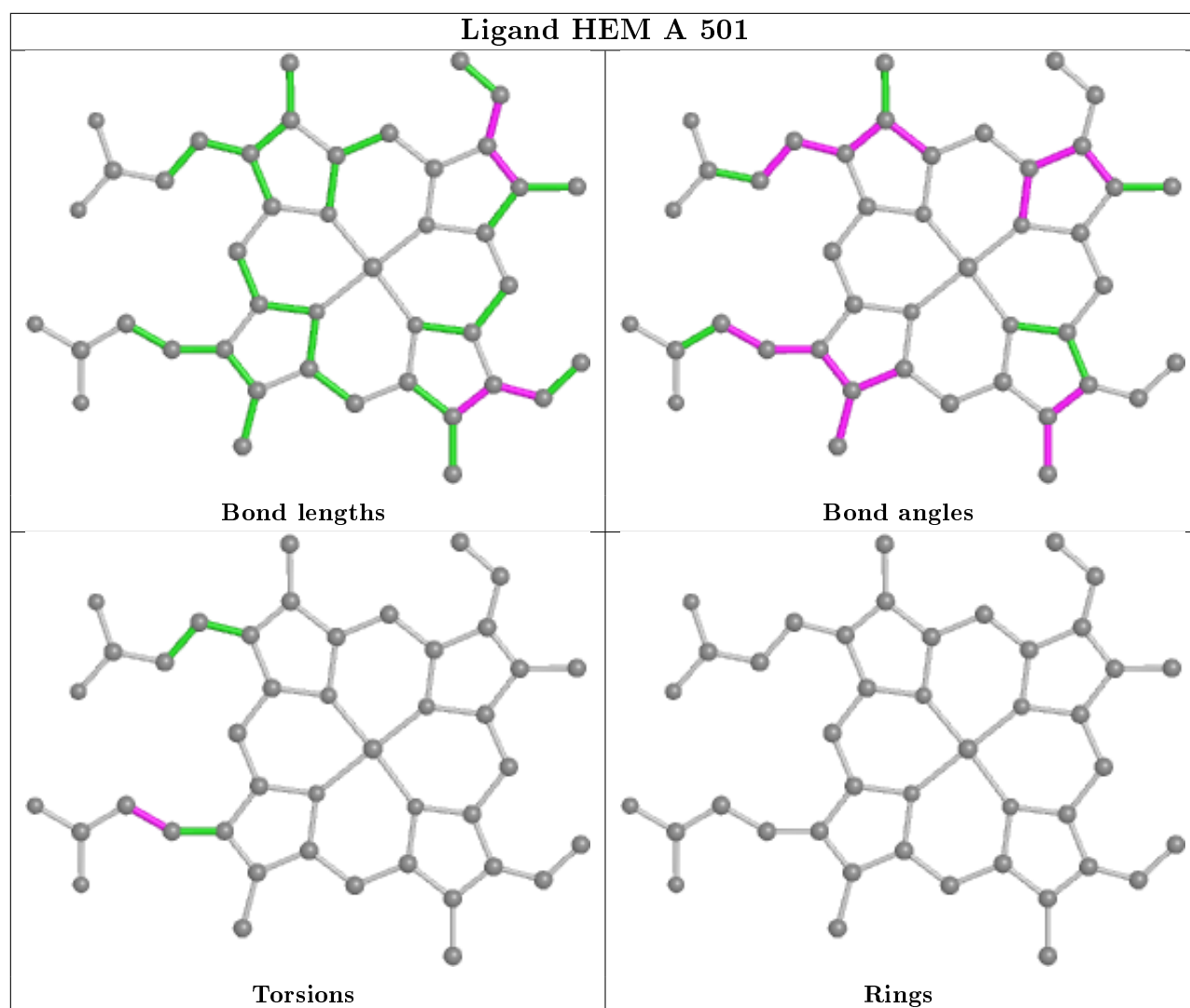


Ligand BBJ B 502









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	370/405 (91%)	0.20	6 (1%) 72 77	36, 55, 74, 103	0
1	B	369/405 (91%)	0.29	11 (2%) 50 57	35, 53, 72, 85	0
1	C	369/405 (91%)	0.33	16 (4%) 35 42	37, 60, 79, 97	0
1	D	378/405 (93%)	0.25	10 (2%) 56 63	37, 54, 74, 87	0
All	All	1486/1620 (91%)	0.27	43 (2%) 51 58	35, 55, 75, 103	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	372	SER	5.0
1	D	376	ALA	4.1
1	C	189	GLN	3.8
1	C	360	GLN	3.4
1	D	375	GLU	3.3
1	C	186	LYS	3.3
1	C	381	GLY	3.3
1	D	377	LYS	3.2
1	B	190	MET	3.1
1	A	285	GLY	3.1
1	A	380	GLY	3.0
1	B	314	PRO	3.0
1	D	379	THR	3.0
1	C	190	MET	2.9
1	A	186	LYS	2.9
1	D	378	GLY	2.8
1	A	198	LYS	2.7
1	B	187	ALA	2.6
1	C	191	GLN	2.6
1	D	361	GLN	2.5
1	B	186	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	359	SER	2.5
1	D	373	LYS	2.5
1	C	401	LYS	2.5
1	C	318	GLU	2.5
1	C	384	LEU	2.5
1	B	191	GLN	2.4
1	B	312	SER	2.4
1	C	355	LEU	2.4
1	A	381	GLY	2.4
1	B	73	HIS	2.4
1	B	14	ALA	2.3
1	C	140	ASN	2.3
1	B	319	PHE	2.3
1	C	287	HIS	2.2
1	C	382	THR	2.2
1	B	283	ALA	2.2
1	C	284	GLY	2.1
1	B	182	PRO	2.1
1	C	282	THR	2.1
1	A	180	VAL	2.1
1	D	374	LEU	2.0
1	D	189	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 monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BBJ	A	502	25/25	0.87	0.29	61,68,87,93	0

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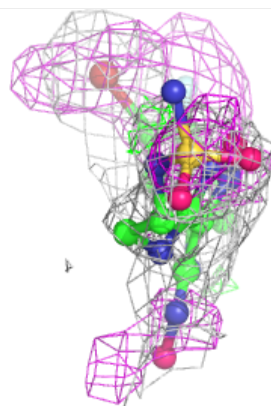
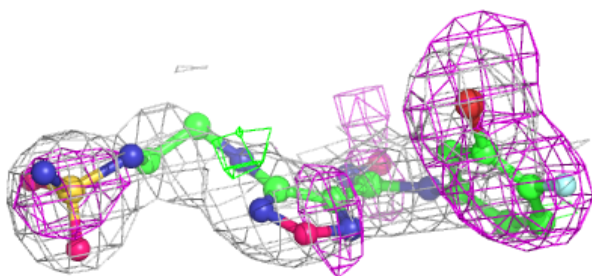
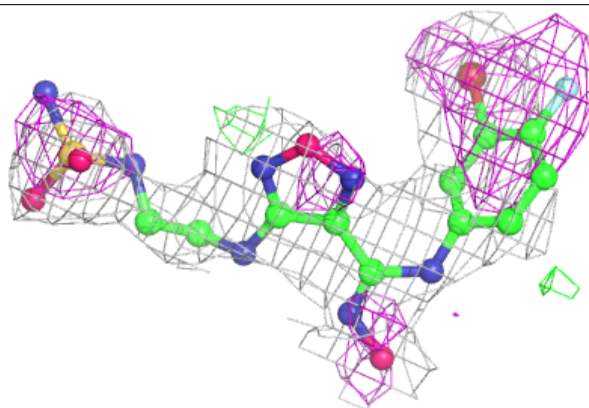
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BBJ	B	502	25/25	0.93	0.19	53,62,83,95	0
3	BBJ	D	502	25/25	0.94	0.15	50,59,84,90	0
2	HEM	C	501	43/43	0.96	0.15	56,62,71,78	0
2	HEM	B	501	43/43	0.97	0.16	47,54,63,73	0
2	HEM	A	501	43/43	0.97	0.14	48,56,68,77	0
2	HEM	D	501	43/43	0.98	0.15	45,50,59,67	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.

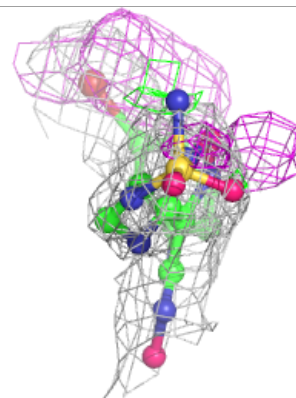
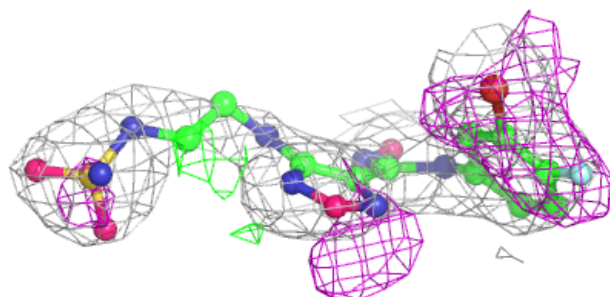
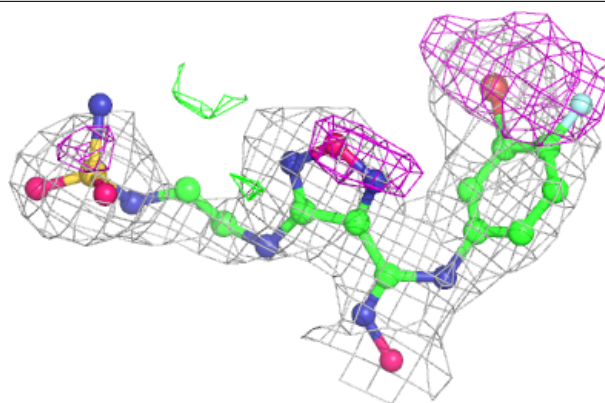
Electron density around BBJ A 502:

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

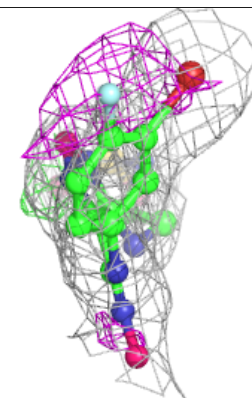
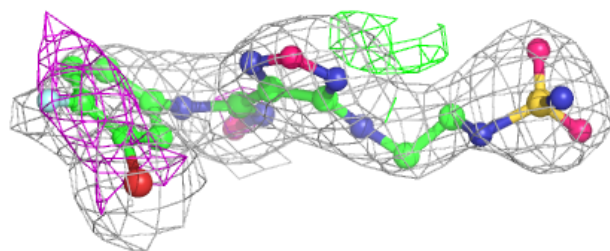
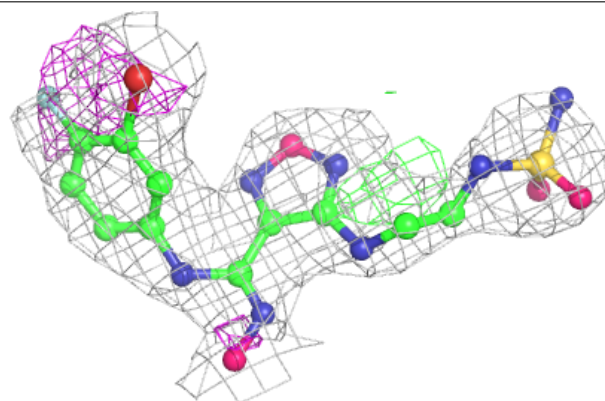


Electron density around BBJ B 502:

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

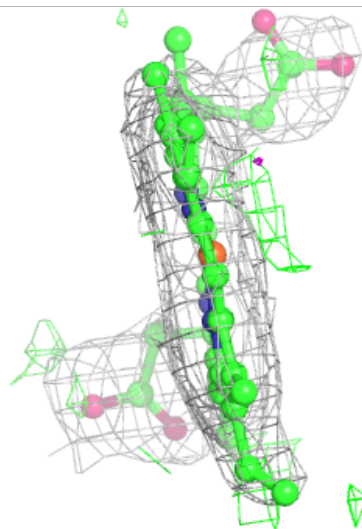
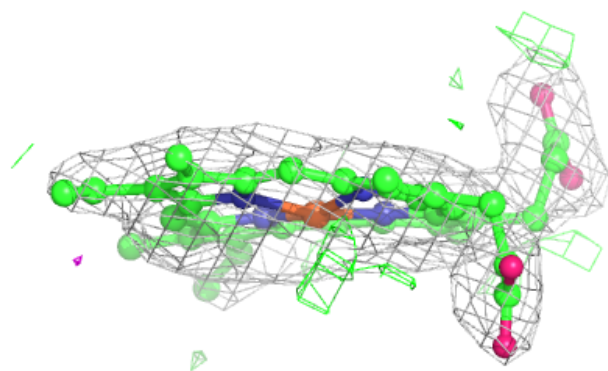
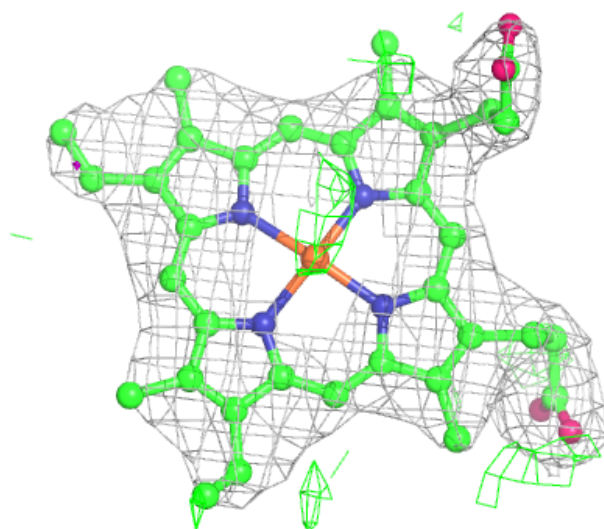
**Electron density around BBJ D 502:**

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



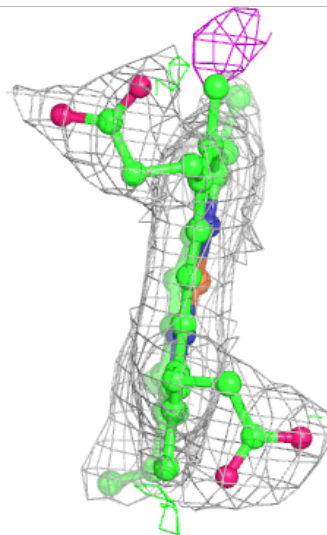
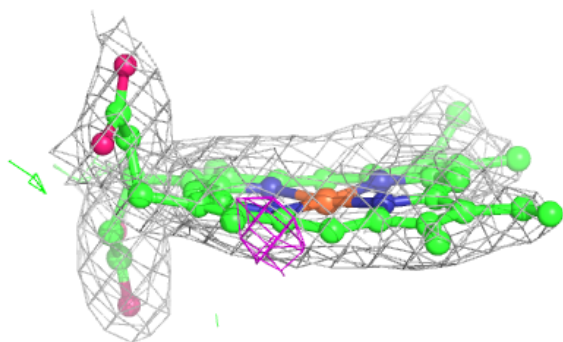
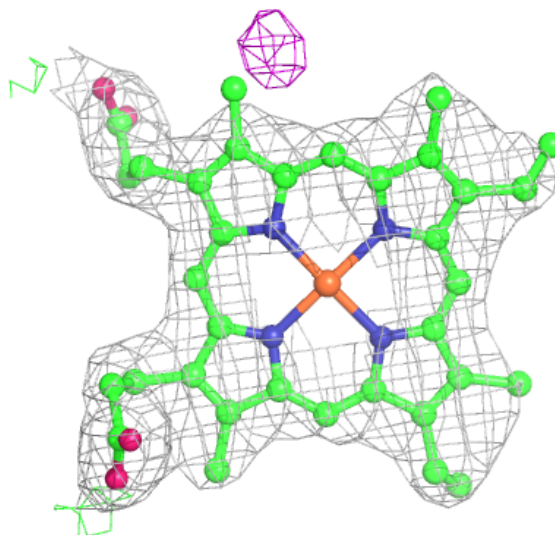
Electron density around HEM C 501:

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



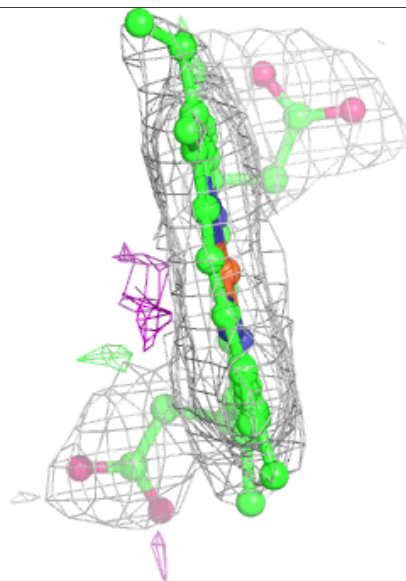
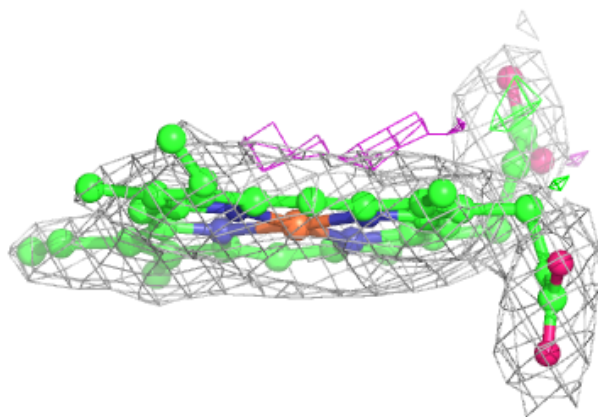
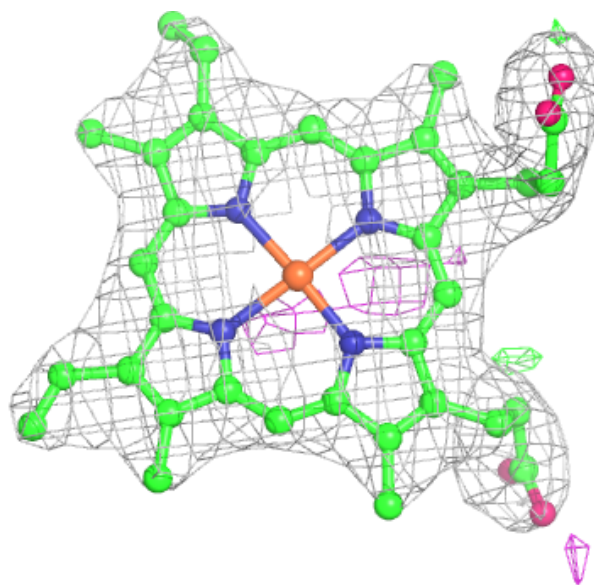
Electron density around HEM B 501:

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



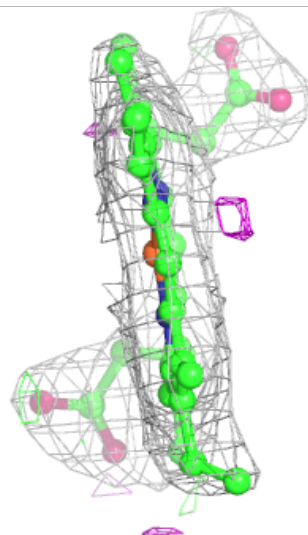
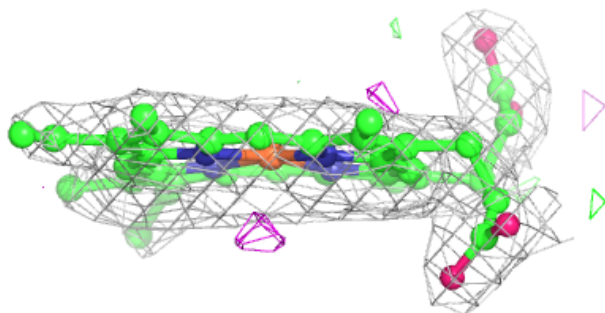
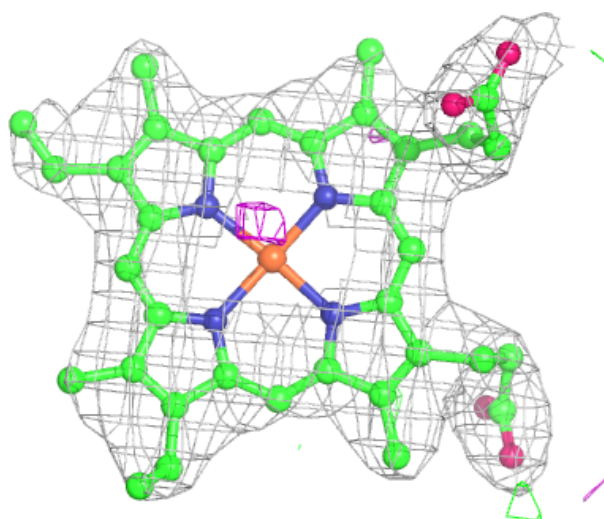
Electron density around HEM A 501:

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



Electron density around HEM D 501:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.