



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:52 PM UTC

PDB ID : 2PG7 / pdb_00002pg7
Title : Crystal Structure of Human Microsomal P450 2A6 N297Q/I300V
Authors : Sansen, S.; Hsu, M.H.; Stout, C.D.; Johnson, E.F.
Deposited on : 2007-04-06
Resolution : 2.80 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)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

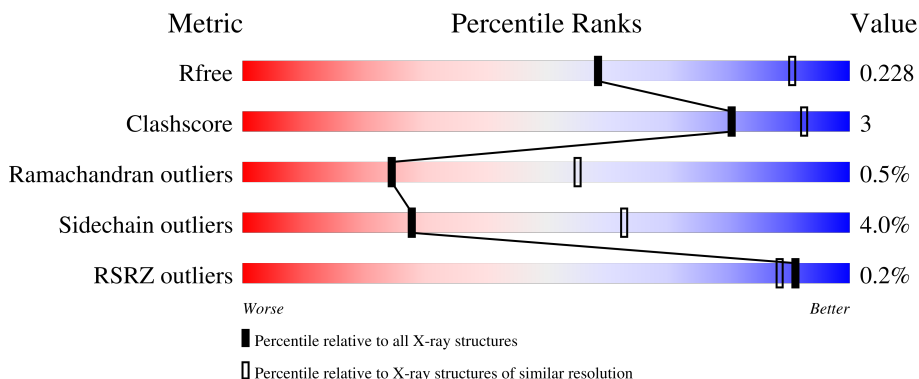
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	476	85% 12% ..
1	B	476	84% 12% ..
1	C	476	84% 12% ..
1	D	476	82% 14% ..

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 15273 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 Cytochrome P450 2A6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	464	3751	2408	648	677	18	0	0	0
1	B	464	3757	2412	650	677	18	0	0	0
1	C	464	3751	2408	648	677	18	0	0	0
1	D	464	3751	2408	648	677	18	0	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	cloning artifact	UNP P11509
A	24	ALA	-	cloning artifact	UNP P11509
A	25	LYS	-	cloning artifact	UNP P11509
A	26	LYS	-	cloning artifact	UNP P11509
A	27	THR	-	cloning artifact	UNP P11509
A	28	SER	-	cloning artifact	UNP P11509
A	160	LEU	HIS	variant	UNP P11509
A	297	GLN	ASN	engineered mutation	UNP P11509
A	300	VAL	ILE	engineered mutation	UNP P11509
A	495	HIS	-	expression tag	UNP P11509
A	496	HIS	-	expression tag	UNP P11509
A	497	HIS	-	expression tag	UNP P11509
A	498	HIS	-	expression tag	UNP P11509
B	23	MET	-	cloning artifact	UNP P11509
B	24	ALA	-	cloning artifact	UNP P11509
B	25	LYS	-	cloning artifact	UNP P11509
B	26	LYS	-	cloning artifact	UNP P11509
B	27	THR	-	cloning artifact	UNP P11509
B	28	SER	-	cloning artifact	UNP P11509
B	160	LEU	HIS	variant	UNP P11509
B	297	GLN	ASN	engineered mutation	UNP P11509

Continued on next page...

Continued from previous page...


Chain	Residue	Modelled	Actual	Comment	Reference
B	300	VAL	ILE	engineered mutation	UNP P11509
B	495	HIS	-	expression tag	UNP P11509
B	496	HIS	-	expression tag	UNP P11509
B	497	HIS	-	expression tag	UNP P11509
B	498	HIS	-	expression tag	UNP P11509
C	23	MET	-	cloning artifact	UNP P11509
C	24	ALA	-	cloning artifact	UNP P11509
C	25	LYS	-	cloning artifact	UNP P11509
C	26	LYS	-	cloning artifact	UNP P11509
C	27	THR	-	cloning artifact	UNP P11509
C	28	SER	-	cloning artifact	UNP P11509
C	160	LEU	HIS	variant	UNP P11509
C	297	GLN	ASN	engineered mutation	UNP P11509
C	300	VAL	ILE	engineered mutation	UNP P11509
C	495	HIS	-	expression tag	UNP P11509
C	496	HIS	-	expression tag	UNP P11509
C	497	HIS	-	expression tag	UNP P11509
C	498	HIS	-	expression tag	UNP P11509
D	23	MET	-	cloning artifact	UNP P11509
D	24	ALA	-	cloning artifact	UNP P11509
D	25	LYS	-	cloning artifact	UNP P11509
D	26	LYS	-	cloning artifact	UNP P11509
D	27	THR	-	cloning artifact	UNP P11509
D	28	SER	-	cloning artifact	UNP P11509
D	160	LEU	HIS	variant	UNP P11509
D	297	GLN	ASN	engineered mutation	UNP P11509
D	300	VAL	ILE	engineered mutation	UNP P11509
D	495	HIS	-	expression tag	UNP P11509
D	496	HIS	-	expression tag	UNP P11509
D	497	HIS	-	expression tag	UNP P11509
D	498	HIS	-	expression tag	UNP P11509

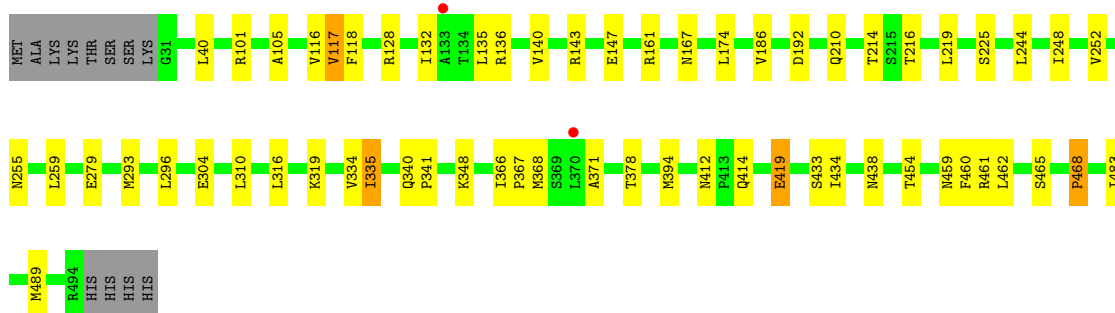
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

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.

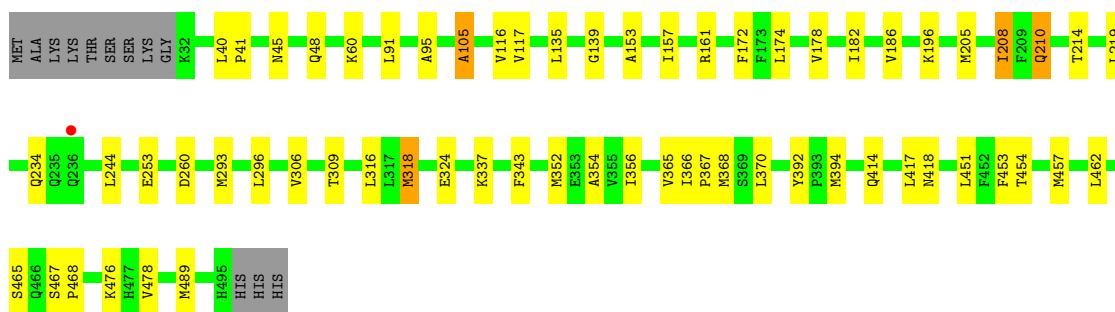
- Molecule 1: Cytochrome P450 2A6

Chain A:  85% 12% ..




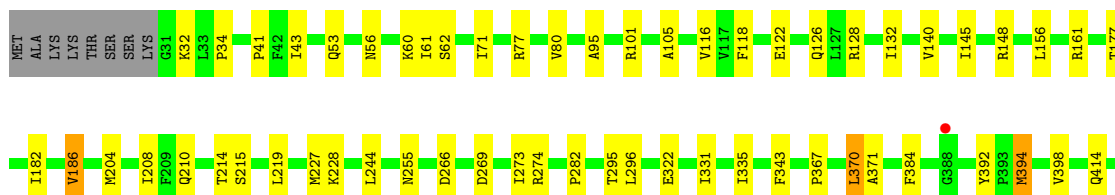
- Molecule 1: Cytochrome P450 2A6

Chain B:  84% 12% ..



- Molecule 1: Cytochrome P450 2A6

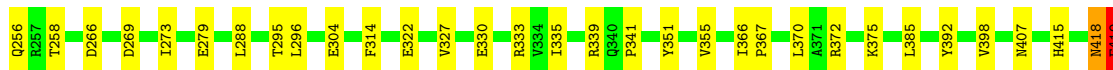
Chain C:  84% 12% ..





- Molecule 1: Cytochrome P450 2A6

Chain D: 82% 14% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.89Å 159.39Å 104.10Å 90.00° 91.92° 90.00°	Depositor
Resolution (Å)	40.00 – 2.80 40.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.00-2.80) 99.5 (40.00-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.81Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.235 , 0.289 0.227 , 0.228	Depositor DCC
R_{free} test set	2865 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	52.3	Xtrriage
Anisotropy	0.849	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.041 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15273	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.68	0/3842	1.16	18/5175 (0.3%)
1	B	0.73	3/3849 (0.1%)	1.16	16/5185 (0.3%)
1	C	0.71	2/3842 (0.1%)	1.16	15/5175 (0.3%)
1	D	0.70	1/3842 (0.0%)	1.16	20/5175 (0.4%)
All	All	0.71	6/15375 (0.0%)	1.16	69/20710 (0.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	205	MET	SD-CE	-8.78	1.57	1.79
1	C	394	MET	SD-CE	-7.22	1.61	1.79
1	B	318	MET	SD-CE	-6.84	1.62	1.79
1	D	34	PRO	CA-C	6.31	1.55	1.51
1	B	293	MET	SD-CE	-5.61	1.65	1.79
1	C	34	PRO	CA-C	5.13	1.54	1.51

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	419	GLU	N-CA-C	-9.14	102.25	113.41
1	A	105	ALA	N-CA-C	8.04	121.06	111.33
1	A	117	VAL	N-CA-C	7.69	117.76	110.53
1	D	186	VAL	N-CA-C	7.63	119.32	111.00
1	B	476	LYS	N-CA-C	-7.43	102.16	112.12
1	B	139	GLY	N-CA-C	7.30	125.51	115.00
1	C	186	VAL	N-CA-C	7.15	117.94	110.72
1	A	118	PHE	N-CA-C	7.11	120.83	112.72
1	C	118	PHE	N-CA-C	6.82	120.49	112.72
1	A	334	VAL	N-CA-C	6.79	117.40	110.82
1	C	116	VAL	N-CA-C	6.59	118.14	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	266	ASP	N-CA-C	6.54	116.69	108.45
1	D	480	PHE	N-CA-C	-6.48	104.30	111.36
1	B	161	ARG	N-CA-C	-6.31	103.93	111.69
1	B	367	PRO	N-CA-C	6.27	122.11	113.65
1	B	219	LEU	N-CA-C	-6.25	104.36	112.23
1	A	367	PRO	N-CA-C	6.21	122.17	113.53
1	A	304	GLU	N-CA-C	6.14	119.87	112.38
1	C	367	PRO	N-CA-C	6.08	121.98	113.53
1	A	465	SER	N-CA-C	-6.04	105.73	114.12
1	A	366	ILE	CA-C-N	6.03	125.75	119.05
1	A	366	ILE	C-N-CA	6.03	125.75	119.05
1	B	186	VAL	N-CA-C	5.95	117.89	111.58
1	D	219	LEU	N-CA-C	-5.94	104.75	112.23
1	B	343	PHE	N-CA-C	5.91	119.31	111.75
1	C	370	LEU	N-CA-C	-5.87	97.75	108.02
1	A	219	LEU	N-CA-C	-5.83	104.88	112.23
1	C	95	ALA	N-CA-C	5.83	118.11	111.11
1	D	266	ASP	N-CA-C	5.76	115.89	108.34
1	A	161	ARG	N-CA-C	-5.75	105.76	112.89
1	D	385	LEU	CA-C-N	5.74	125.70	119.78
1	D	385	LEU	C-N-CA	5.74	125.70	119.78
1	D	143	ARG	N-CA-C	5.74	117.54	111.28
1	C	343	PHE	N-CA-C	5.61	118.16	111.71
1	D	95	ALA	N-CA-C	5.61	117.86	111.02
1	B	91	LEU	N-CA-C	5.60	119.37	112.54
1	B	172	PHE	N-CA-C	5.58	119.70	113.01
1	B	366	ILE	CA-C-N	5.57	125.41	119.28
1	B	366	ILE	C-N-CA	5.57	125.41	119.28
1	D	168	ILE	N-CA-C	5.52	118.06	108.95
1	A	116	VAL	N-CA-C	5.52	116.25	110.62
1	D	304	GLU	N-CA-C	5.49	118.02	111.71
1	C	398	VAL	N-CA-C	-5.48	105.03	111.00
1	B	105	ALA	N-CA-C	5.44	122.39	110.80
1	D	370	LEU	N-CA-C	-5.44	99.42	108.34
1	C	219	LEU	N-CA-C	-5.40	105.43	112.23
1	A	460	PHE	N-CA-C	5.38	118.01	109.50
1	C	62	SER	N-CA-C	-5.38	105.45	112.23
1	C	105	ALA	N-CA-C	5.36	120.21	111.37
1	D	341	PRO	N-CA-C	5.34	119.59	111.15
1	B	451	LEU	N-CA-C	5.31	117.14	111.36
1	A	419	GLU	N-CA-C	5.28	117.78	111.71
1	D	288	LEU	N-CA-C	5.25	117.42	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	367	PRO	N-CA-C	5.25	120.66	113.84
1	C	161	ARG	N-CA-C	-5.23	105.18	112.45
1	B	95	ALA	N-CA-C	5.22	119.98	111.37
1	A	186	VAL	N-CA-C	5.19	119.67	112.35
1	B	370	LEU	N-CA-C	-5.18	100.08	108.52
1	D	33	LEU	N-CA-C	-5.14	102.73	110.24
1	D	460	PHE	N-CA-C	5.13	117.79	109.06
1	D	398	VAL	N-CA-C	-5.11	106.17	111.58
1	A	461	ARG	N-CA-C	-5.09	101.39	109.59
1	A	483	ILE	N-CA-C	5.08	113.65	107.61
1	A	454	THR	N-CA-C	5.07	116.50	111.07
1	C	227	MET	N-CA-C	5.06	118.55	112.38
1	D	366	ILE	CA-C-N	5.05	124.72	119.56
1	D	366	ILE	C-N-CA	5.05	124.72	119.56
1	B	116	VAL	N-CA-C	5.04	115.81	110.72
1	C	461	ARG	N-CA-C	-5.03	101.95	109.95

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	3751	0	3734	19	0
1	B	3757	0	3738	18	0
1	C	3751	0	3734	16	0
1	D	3751	0	3734	27	0
2	A	43	0	30	2	0
2	B	43	0	30	1	0
2	C	43	0	30	0	0
2	D	43	0	30	2	0
3	A	20	0	0	0	0
3	B	23	0	0	0	0
3	C	25	0	0	0	0
3	D	23	0	0	0	0
All	All	15273	0	15060	78	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 3.

All (78) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:MET:HE3	1:B:454:THR:HG22	1.70	0.74
1:D:145:ILE:HD13	1:D:185:ILE:HD11	1.75	0.69
1:C:32:LYS:HB3	1:C:384:PHE:HB3	1.75	0.67
1:D:462:LEU:HD22	1:D:489:MET:HE1	1.76	0.66
1:D:244:LEU:HB3	1:D:296:LEU:HD11	1.79	0.64
1:B:324:GLU:HG3	1:B:457:MET:HE1	1.81	0.63
1:B:368:MET:HG2	1:B:394:MET:SD	2.40	0.62
1:A:244:LEU:HB3	1:A:296:LEU:HD11	1.83	0.60
1:D:101:ARG:HD3	1:D:117:VAL:O	2.01	0.60
1:D:117:VAL:HG22	2:D:500:HEM:HAD1	1.84	0.60
1:C:128:ARG:HE	1:C:132:ILE:HD11	1.67	0.59
1:B:462:LEU:HD22	1:B:489:MET:HE1	1.88	0.56
1:D:335:ILE:HA	1:D:339:ARG:HH21	1.70	0.56
1:A:132:ILE:HG22	1:A:136:ARG:NH1	2.21	0.55
1:C:53:GLN:HB3	1:C:56:ASN:HB2	1.89	0.55
1:A:40:LEU:HD21	1:C:43:ILE:HD13	1.89	0.55
1:A:225:SER:HB2	1:D:225:SER:HB2	1.88	0.55
1:A:433:SER:HB3	2:A:500:HEM:HBA1	1.89	0.54
1:C:156:LEU:HB2	1:C:177:THR:HG21	1.90	0.54
1:D:407:ASN:H	1:D:415:HIS:HE1	1.55	0.53
1:A:462:LEU:HD22	1:A:489:MET:HE1	1.90	0.53
1:D:419:GLU:H	1:D:419:GLU:CD	2.17	0.52
1:A:128:ARG:O	1:A:132:ILE:HG13	2.08	0.52
1:D:140:VAL:HG22	1:D:444:LEU:HD13	1.92	0.52
1:D:433:SER:HB3	2:D:500:HEM:HBA1	1.92	0.52
1:D:204:MET:O	1:D:208:ILE:HG12	2.11	0.51
1:D:330:GLU:HG3	1:D:333:ARG:NH2	2.27	0.50
1:B:244:LEU:HB3	1:B:296:LEU:HD11	1.94	0.50
1:C:269:ASP:O	1:C:273:ILE:HG12	2.11	0.50
1:D:269:ASP:O	1:D:273:ILE:HG12	2.11	0.49
1:A:412:ASN:HD21	1:A:414:GLN:HB2	1.78	0.49
1:C:214:THR:HG22	1:C:215:SER:H	1.77	0.49
1:A:248:ILE:O	1:A:252:VAL:HG23	2.13	0.49
1:B:318:MET:HE3	1:B:462:LEU:HB3	1.94	0.49
1:B:153:ALA:O	1:B:157:ILE:HG12	2.13	0.49
1:B:45:ASN:HD22	1:B:48:GLN:NE2	2.10	0.49
1:A:132:ILE:HG22	1:A:136:ARG:HH12	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:GLN:NE2	1:B:417:LEU:HD23	2.29	0.48
1:C:77:ARG:HH11	1:C:77:ARG:HG2	1.78	0.48
1:C:122:GLU:O	1:C:126:GLN:HB2	2.15	0.47
1:D:189:ASP:CG	1:D:190:ARG:H	2.23	0.47
1:D:466:GLN:HG3	1:D:471:ILE:HG12	1.96	0.47
1:D:157:ILE:HG21	1:D:459:ASN:HD22	1.80	0.47
1:D:351:TYR:O	1:D:355:VAL:HG23	2.15	0.47
1:C:186:VAL:HG13	1:C:295:THR:HG23	1.96	0.46
1:C:331:ILE:HG23	1:C:335:ILE:HD12	1.97	0.46
1:C:80:VAL:HG13	1:C:394:MET:HE3	1.97	0.46
1:B:352:MET:O	1:B:356:ILE:HG12	2.17	0.45
1:B:117:VAL:HG22	2:B:500:HEM:HAD1	1.98	0.45
1:A:210:GLN:O	1:A:214:THR:HG23	2.16	0.45
1:B:318:MET:HE1	1:B:489:MET:HB2	1.99	0.44
1:B:210:GLN:O	1:B:214:THR:HG23	2.17	0.44
1:A:117:VAL:HG22	2:A:500:HEM:HAD1	2.00	0.44
1:B:178:VAL:HG11	1:B:306:VAL:HB	2.00	0.44
1:C:244:LEU:HB3	1:C:296:LEU:HD11	1.98	0.44
1:D:33:LEU:HD11	1:D:77:ARG:NH1	2.33	0.44
1:D:57:SER:O	1:D:61:ILE:HG12	2.18	0.44
1:D:457:MET:HE1	1:D:462:LEU:HD21	2.00	0.44
1:C:204:MET:O	1:C:208:ILE:HG12	2.17	0.43
1:D:148:ARG:HH21	1:D:190:ARG:HB3	1.83	0.43
1:A:319:LYS:HD2	1:A:468:PRO:O	2.18	0.43
1:A:335:ILE:HG21	1:A:341:PRO:HG3	2.00	0.43
1:A:143:ARG:O	1:A:147:GLU:HG2	2.19	0.42
1:B:208:ILE:HD13	1:B:208:ILE:HA	1.93	0.42
1:D:186:VAL:HG13	1:D:295:THR:HG23	2.02	0.42
1:C:214:THR:HG22	1:C:215:SER:N	2.34	0.42
1:B:453:PHE:O	1:B:457:MET:HG2	2.20	0.41
1:D:372:ARG:HH22	1:D:435:GLY:HA3	1.84	0.41
1:A:368:MET:HG2	1:A:394:MET:SD	2.60	0.41
1:B:309:THR:OG1	1:B:365:VAL:HG21	2.20	0.41
1:C:101:ARG:NH2	1:C:370:LEU:O	2.53	0.41
1:D:314:PHE:HE2	1:D:457:MET:HE3	1.86	0.41
1:A:174:LEU:HD22	1:A:310:LEU:HD13	2.03	0.41
1:D:135:LEU:HG	1:D:140:VAL:HG21	2.03	0.41
1:D:314:PHE:CE2	1:D:457:MET:HE3	2.55	0.41
1:A:101:ARG:HD2	1:A:117:VAL:O	2.22	0.40
1:B:354:ALA:HB2	1:B:417:LEU:HD13	2.03	0.40
1:A:255:ASN:O	1:A:259:LEU:HB2	2.21	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	462/476 (97%)	436 (94%)	23 (5%)	3 (1%)	21	51
1	B	462/476 (97%)	429 (93%)	31 (7%)	2 (0%)	30	60
1	C	462/476 (97%)	440 (95%)	19 (4%)	3 (1%)	21	51
1	D	462/476 (97%)	430 (93%)	30 (6%)	2 (0%)	30	60
All	All	1848/1904 (97%)	1735 (94%)	103 (6%)	10 (0%)	24	55

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	VAL
1	C	371	ALA
1	A	371	ALA
1	B	468	PRO
1	A	438	ASN
1	B	105	ALA
1	C	282	PRO
1	D	418	ASN
1	D	468	PRO
1	C	140	VAL

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	411/422 (97%)	396 (96%)	15 (4%)	31	66
1	B	412/422 (98%)	393 (95%)	19 (5%)	24	58
1	C	411/422 (97%)	394 (96%)	17 (4%)	27	62
1	D	411/422 (97%)	397 (97%)	14 (3%)	32	68
All	All	1645/1688 (98%)	1580 (96%)	65 (4%)	28	63

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	LEU
1	A	167	ASN
1	A	192	ASP
1	A	216	THR
1	A	279	GLU
1	A	293	MET
1	A	316	LEU
1	A	335	ILE
1	A	340	GLN
1	A	348	LYS
1	A	378	THR
1	A	419	GLU
1	A	434	ILE
1	A	459	ASN
1	A	468	PRO
1	B	40	LEU
1	B	41	PRO
1	B	60	LYS
1	B	135	LEU
1	B	174	LEU
1	B	182	ILE
1	B	196	LYS
1	B	208	ILE
1	B	210	GLN
1	B	234	GLN
1	B	253	GLU
1	B	260	ASP
1	B	316	LEU
1	B	337	LYS
1	B	392	TYR
1	B	418	ASN
1	B	465	SER
1	B	467	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	478	VAL
1	C	41	PRO
1	C	60	LYS
1	C	61	ILE
1	C	71	ILE
1	C	145	ILE
1	C	148	ARG
1	C	182	ILE
1	C	210	GLN
1	C	228	LYS
1	C	255	ASN
1	C	274	ARG
1	C	322	GLU
1	C	392	TYR
1	C	414	GLN
1	C	417	LEU
1	C	420	LYS
1	C	434	ILE
1	D	40	LEU
1	D	41	PRO
1	D	168	ILE
1	D	174	LEU
1	D	256	GLN
1	D	258	THR
1	D	279	GLU
1	D	322	GLU
1	D	327	VAL
1	D	375	LYS
1	D	392	TYR
1	D	418	ASN
1	D	419	GLU
1	D	434	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	53	GLN
1	A	56	ASN
1	A	104	GLN
1	A	210	GLN
1	A	236	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	407	ASN
1	A	409	GLN
1	A	412	ASN
1	A	414	GLN
1	A	466	GLN
1	B	48	GLN
1	B	104	GLN
1	B	255	ASN
1	B	340	GLN
1	B	418	ASN
1	B	422	GLN
1	B	438	ASN
1	C	53	GLN
1	C	56	ASN
1	C	150	GLN
1	C	167	ASN
1	C	255	ASN
1	C	276	GLN
1	D	72	HIS
1	D	104	GLN
1	D	126	GLN
1	D	236	GLN
1	D	256	GLN
1	D	340	GLN
1	D	458	GLN
1	D	477	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 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	500	1	50,50,50	2.52	24 (48%)	67,82,82	1.47	13 (19%)
2	HEM	B	500	1	50,50,50	2.49	25 (50%)	67,82,82	1.46	13 (19%)
2	HEM	C	500	1	50,50,50	2.48	24 (48%)	67,82,82	1.40	14 (20%)
2	HEM	A	500	1	50,50,50	2.55	24 (48%)	67,82,82	1.53	13 (19%)

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	500	1	-	4/14/54/54	-
2	HEM	B	500	1	-	4/14/54/54	-
2	HEM	C	500	1	-	6/14/54/54	-
2	HEM	A	500	1	-	4/14/54/54	-

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C1D-ND	-5.42	1.28	1.38
2	B	500	HEM	C4A-NA	-5.28	1.29	1.39
2	D	500	HEM	C1D-ND	-5.25	1.28	1.38
2	A	500	HEM	C4A-NA	-5.22	1.29	1.39
2	B	500	HEM	C1D-ND	-5.21	1.28	1.38
2	C	500	HEM	C1D-ND	-5.18	1.28	1.38
2	A	500	HEM	C1B-NB	-5.11	1.31	1.40
2	D	500	HEM	C4A-NA	-4.85	1.30	1.39
2	D	500	HEM	C1B-NB	-4.82	1.31	1.40
2	C	500	HEM	C4A-NA	-4.71	1.30	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C1B-NB	-4.67	1.32	1.40
2	C	500	HEM	C1C-NC	-4.36	1.31	1.39
2	C	500	HEM	C1B-NB	-4.36	1.32	1.40
2	B	500	HEM	C1C-NC	-4.35	1.31	1.39
2	A	500	HEM	C1C-NC	-4.21	1.31	1.39
2	A	500	HEM	C4B-NB	-4.15	1.30	1.38
2	D	500	HEM	CAC-C3C	-4.09	1.36	1.47
2	B	500	HEM	C4B-NB	-4.09	1.30	1.38
2	A	500	HEM	C1C-C2C	-4.04	1.37	1.45
2	D	500	HEM	C1C-NC	-4.00	1.32	1.39
2	B	500	HEM	C4D-ND	-3.99	1.33	1.40
2	C	500	HEM	C4D-ND	-3.97	1.33	1.40
2	A	500	HEM	FE-NB	3.91	2.06	1.94
2	A	500	HEM	CBB-CAB	3.90	1.49	1.30
2	D	500	HEM	CBB-CAB	3.89	1.49	1.30
2	B	500	HEM	FE-ND	3.89	2.06	1.94
2	C	500	HEM	C4B-NB	-3.87	1.31	1.38
2	D	500	HEM	FE-ND	3.87	2.06	1.94
2	B	500	HEM	CBB-CAB	3.87	1.49	1.30
2	C	500	HEM	CBB-CAB	3.85	1.48	1.30
2	A	500	HEM	CAC-C3C	-3.77	1.37	1.47
2	D	500	HEM	C4B-NB	-3.77	1.31	1.38
2	C	500	HEM	C1C-C2C	-3.76	1.37	1.45
2	C	500	HEM	FE-ND	3.74	2.06	1.94
2	D	500	HEM	CMA-C3A	3.71	1.58	1.50
2	B	500	HEM	CAC-C3C	-3.71	1.37	1.47
2	A	500	HEM	FE-ND	3.61	2.06	1.94
2	D	500	HEM	C4D-ND	-3.56	1.34	1.40
2	C	500	HEM	FE-NB	3.56	2.05	1.94
2	C	500	HEM	CAC-C3C	-3.55	1.37	1.47
2	D	500	HEM	C1C-C2C	-3.49	1.38	1.45
2	A	500	HEM	C4D-ND	-3.47	1.34	1.40
2	A	500	HEM	CMA-C3A	3.38	1.57	1.50
2	D	500	HEM	FE-NB	3.31	2.05	1.94
2	B	500	HEM	FE-NB	3.28	2.05	1.94
2	C	500	HEM	FE-NA	3.27	2.06	1.95
2	D	500	HEM	FE-NA	3.27	2.06	1.95
2	C	500	HEM	CMA-C3A	3.26	1.57	1.50
2	A	500	HEM	O2A-CGA	-3.25	1.20	1.30
2	D	500	HEM	C4C-NC	-3.19	1.33	1.39
2	B	500	HEM	CMA-C3A	3.03	1.57	1.50
2	C	500	HEM	C4C-NC	-3.00	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C4C-NC	-3.00	1.34	1.39
2	C	500	HEM	O2A-CGA	-2.98	1.20	1.30
2	B	500	HEM	O2A-CGA	-2.95	1.21	1.30
2	D	500	HEM	O2A-CGA	-2.90	1.21	1.30
2	B	500	HEM	C1C-C2C	-2.90	1.39	1.45
2	B	500	HEM	FE-NA	2.86	2.04	1.95
2	D	500	HEM	C3B-C2B	2.85	1.43	1.37
2	D	500	HEM	C3C-C4C	-2.78	1.41	1.46
2	A	500	HEM	FE-NA	2.77	2.04	1.95
2	D	500	HEM	CMC-C2C	2.69	1.56	1.50
2	B	500	HEM	CMC-C2C	2.68	1.56	1.50
2	A	500	HEM	C4D-C3D	-2.65	1.40	1.45
2	C	500	HEM	CMC-C2C	2.64	1.56	1.50
2	A	500	HEM	CMC-C2C	2.61	1.56	1.50
2	C	500	HEM	C3C-C4C	-2.60	1.41	1.46
2	C	500	HEM	C1D-C2D	-2.58	1.39	1.44
2	B	500	HEM	FE-NC	2.57	2.03	1.95
2	C	500	HEM	C3B-C2B	2.53	1.42	1.37
2	D	500	HEM	C4D-C3D	-2.51	1.40	1.45
2	C	500	HEM	CBC-CAC	2.49	1.42	1.30
2	D	500	HEM	CAD-C3D	2.48	1.57	1.51
2	B	500	HEM	CAD-C3D	2.47	1.57	1.51
2	C	500	HEM	FE-NC	2.46	2.03	1.95
2	A	500	HEM	CAD-C3D	2.46	1.57	1.51
2	B	500	HEM	C4C-NC	-2.44	1.35	1.39
2	A	500	HEM	CBC-CAC	2.42	1.42	1.30
2	B	500	HEM	CBC-CAC	2.41	1.42	1.30
2	B	500	HEM	C3C-C4C	-2.40	1.41	1.46
2	A	500	HEM	C3B-C2B	2.39	1.42	1.37
2	D	500	HEM	CBC-CAC	2.34	1.41	1.30
2	C	500	HEM	C1A-C2A	-2.34	1.39	1.44
2	A	500	HEM	FE-NC	2.34	2.02	1.95
2	B	500	HEM	C1D-C2D	-2.31	1.39	1.44
2	A	500	HEM	C1D-C2D	-2.30	1.39	1.44
2	D	500	HEM	C1D-C2D	-2.27	1.39	1.44
2	B	500	HEM	C4D-C3D	-2.27	1.41	1.45
2	D	500	HEM	FE-NC	2.27	2.02	1.95
2	A	500	HEM	CBD-CGD	2.26	1.55	1.50
2	B	500	HEM	CBD-CGD	2.23	1.55	1.50
2	B	500	HEM	C3B-C2B	2.23	1.41	1.37
2	C	500	HEM	CAD-C3D	2.20	1.57	1.51
2	A	500	HEM	C1A-C2A	-2.19	1.40	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	HEM	CBD-CGD	2.16	1.55	1.50
2	B	500	HEM	C1A-C2A	-2.16	1.40	1.44
2	C	500	HEM	C4D-C3D	-2.15	1.41	1.45

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	HEM	CHD-C4C-NC	-4.19	119.89	124.45
2	D	500	HEM	CHB-C1B-NB	-4.09	119.31	124.37
2	B	500	HEM	CHD-C4C-NC	-3.95	120.15	124.45
2	A	500	HEM	C4B-C3B-C2B	-3.44	104.12	107.28
2	B	500	HEM	CHB-C1B-NB	-3.26	120.34	124.37
2	D	500	HEM	C4B-C3B-C2B	-3.24	104.31	107.28
2	A	500	HEM	C3B-C4B-NB	3.13	111.72	109.47
2	D	500	HEM	CHD-C4C-NC	-3.08	121.10	124.45
2	C	500	HEM	CHD-C4C-NC	-3.06	121.12	124.45
2	A	500	HEM	CHB-C1B-NB	-3.05	120.59	124.37
2	C	500	HEM	C4B-C3B-C2B	-3.00	104.52	107.28
2	B	500	HEM	C4B-C3B-C2B	-2.99	104.53	107.28
2	D	500	HEM	C1B-NB-C4B	2.95	108.70	105.21
2	C	500	HEM	C3B-C4B-NB	2.92	111.56	109.47
2	A	500	HEM	C3B-C2B-C1B	-2.91	104.23	106.41
2	A	500	HEM	C1C-CHC-C4B	2.77	131.91	126.02
2	B	500	HEM	CHC-C1C-NC	-2.70	121.52	124.45
2	A	500	HEM	C4D-ND-C1D	2.66	108.36	105.21
2	B	500	HEM	C1B-NB-C4B	2.65	108.35	105.21
2	B	500	HEM	C3B-C2B-C1B	-2.65	104.42	106.41
2	C	500	HEM	C3B-C2B-C1B	-2.62	104.44	106.41
2	D	500	HEM	C4D-ND-C1D	2.61	108.30	105.21
2	D	500	HEM	C3B-C2B-C1B	-2.60	104.46	106.41
2	B	500	HEM	C4D-ND-C1D	2.59	108.27	105.21
2	D	500	HEM	C1C-CHC-C4B	2.58	131.51	126.02
2	B	500	HEM	C4C-C3C-C2C	-2.58	104.58	106.81
2	C	500	HEM	C1B-NB-C4B	2.54	108.22	105.21
2	C	500	HEM	C4D-ND-C1D	2.53	108.20	105.21
2	C	500	HEM	C4C-C3C-C2C	-2.52	104.63	106.81
2	B	500	HEM	C1C-CHC-C4B	2.49	131.31	126.02
2	A	500	HEM	C4C-C3C-C2C	-2.47	104.67	106.81
2	D	500	HEM	C4C-C3C-C2C	-2.47	104.68	106.81
2	D	500	HEM	O2A-CGA-CBA	2.46	121.77	114.00
2	C	500	HEM	C1C-CHC-C4B	2.41	131.13	126.02
2	C	500	HEM	C4C-CHD-C1D	2.36	131.03	126.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	HEM	O2A-CGA-CBA	2.34	121.41	114.00
2	D	500	HEM	C3B-C4B-NB	2.34	111.15	109.47
2	C	500	HEM	C4A-CHB-C1B	2.34	131.75	126.25
2	A	500	HEM	C1B-NB-C4B	2.34	107.97	105.21
2	A	500	HEM	C4A-CHB-C1B	2.24	131.53	126.25
2	B	500	HEM	C3B-C4B-NB	2.23	111.07	109.47
2	A	500	HEM	C4D-C3D-C2D	-2.21	103.68	106.89
2	B	500	HEM	C4D-C3D-C2D	-2.19	103.70	106.89
2	C	500	HEM	CHC-C1C-NC	-2.17	122.09	124.45
2	D	500	HEM	C4D-C3D-C2D	-2.14	103.78	106.89
2	B	500	HEM	O2A-CGA-CBA	2.10	120.64	114.00
2	C	500	HEM	CHB-C1B-NB	-2.09	121.78	124.37
2	C	500	HEM	O2A-CGA-CBA	2.08	120.58	114.00
2	C	500	HEM	C4D-C3D-C2D	-2.06	103.90	106.89
2	D	500	HEM	CHD-C4C-C3C	2.03	128.63	125.21
2	D	500	HEM	C4A-CHB-C1B	2.03	131.01	126.25
2	B	500	HEM	C4A-CHB-C1B	2.03	131.01	126.25
2	A	500	HEM	CAD-C3D-C4D	2.02	128.21	124.70

There are no chirality outliers.

All (18) torsion outliers are listed below:

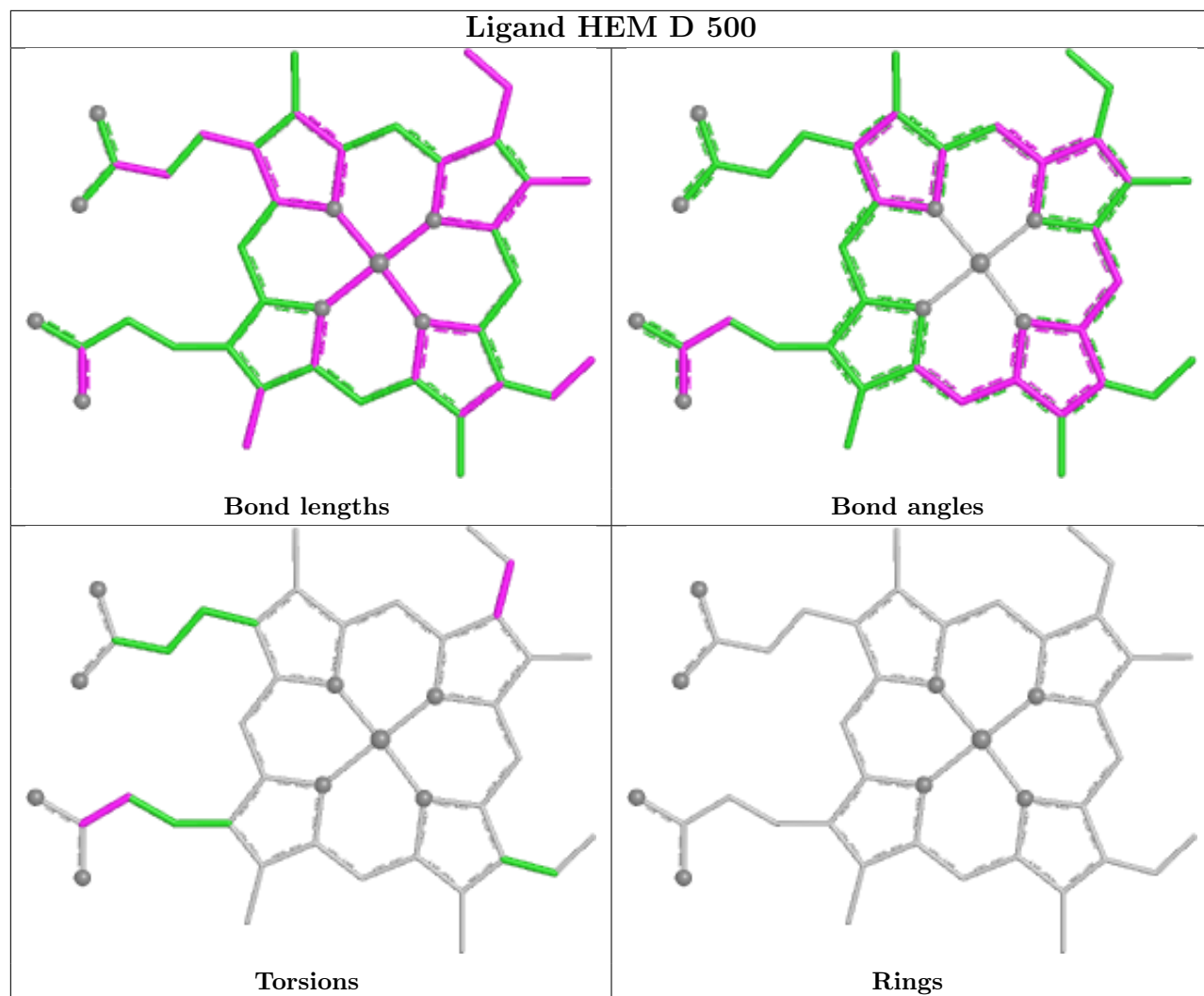
Mol	Chain	Res	Type	Atoms
2	A	500	HEM	C2C-C3C-CAC-CBC
2	C	500	HEM	C2C-C3C-CAC-CBC
2	D	500	HEM	C2C-C3C-CAC-CBC
2	A	500	HEM	C4C-C3C-CAC-CBC
2	C	500	HEM	C4C-C3C-CAC-CBC
2	D	500	HEM	C4C-C3C-CAC-CBC
2	B	500	HEM	C2C-C3C-CAC-CBC
2	B	500	HEM	CAA-CBA-CGA-O2A
2	C	500	HEM	CAD-CBD-CGD-O1D
2	B	500	HEM	CAA-CBA-CGA-O1A
2	C	500	HEM	CAD-CBD-CGD-O2D
2	C	500	HEM	CAA-CBA-CGA-O2A
2	C	500	HEM	CAA-CBA-CGA-O1A
2	D	500	HEM	CAA-CBA-CGA-O1A
2	D	500	HEM	CAA-CBA-CGA-O2A
2	A	500	HEM	CAA-CBA-CGA-O1A
2	A	500	HEM	CAA-CBA-CGA-O2A
2	B	500	HEM	C4C-C3C-CAC-CBC

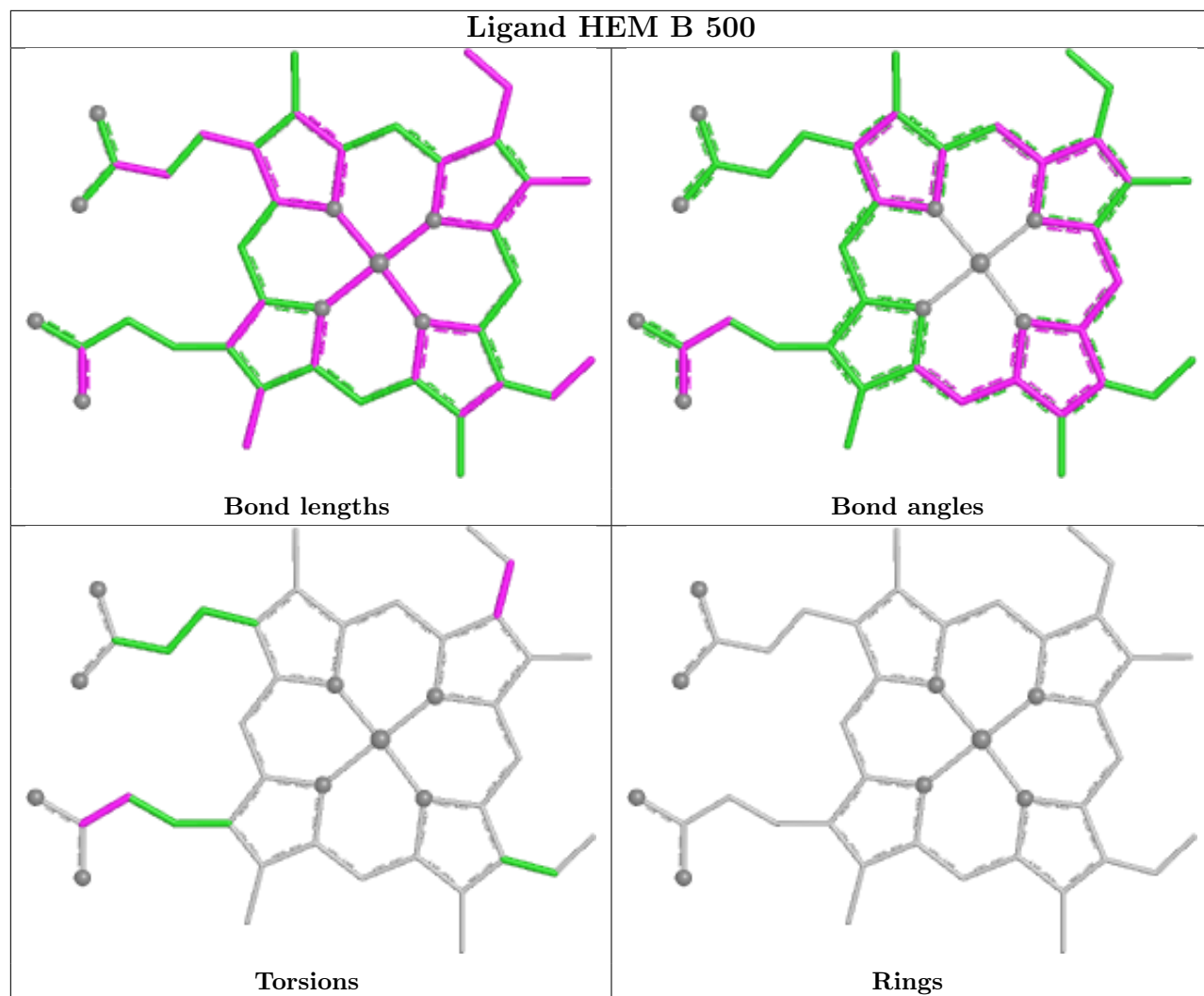
There are no ring outliers.

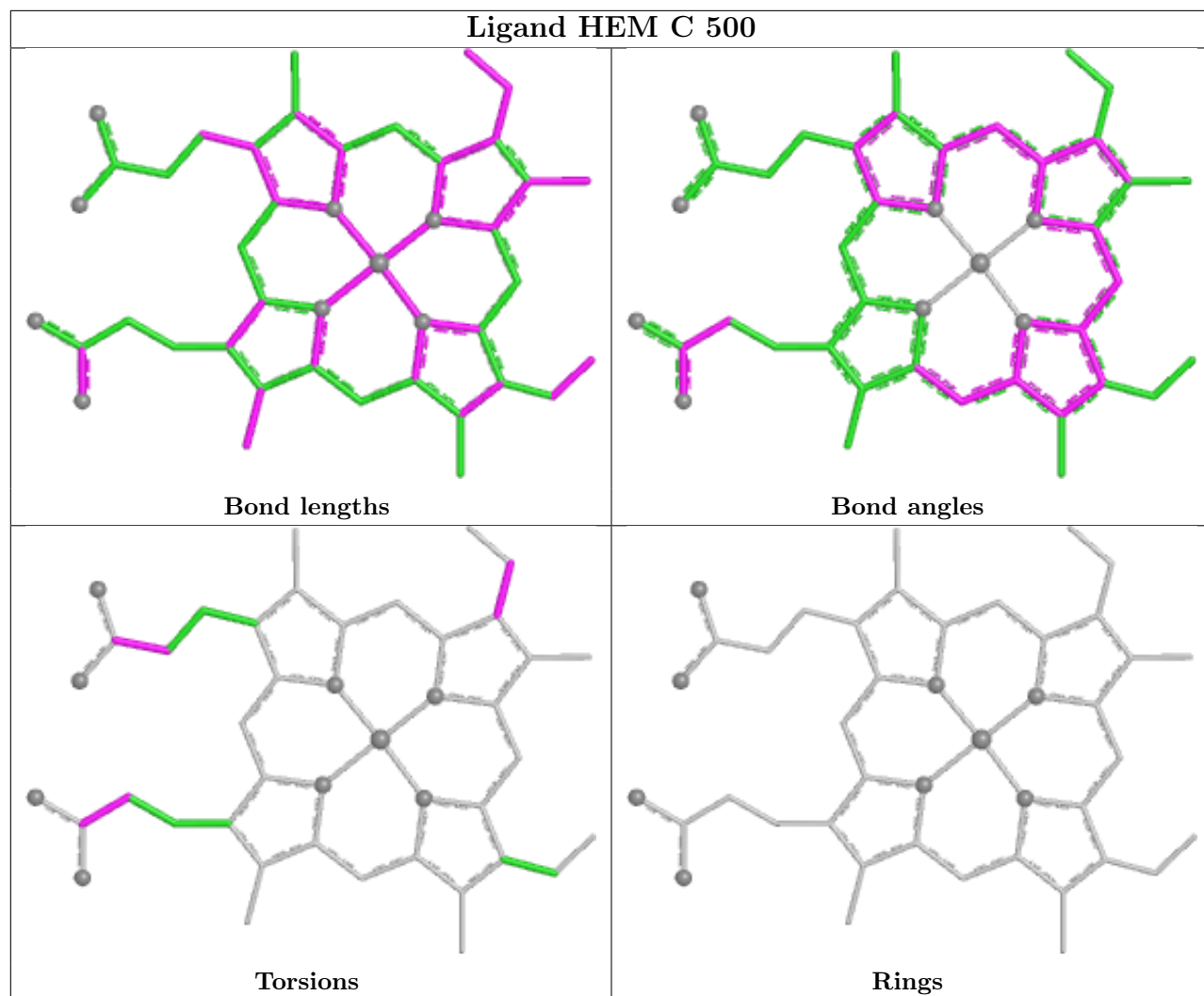
3 monomers are involved in 5 short contacts:

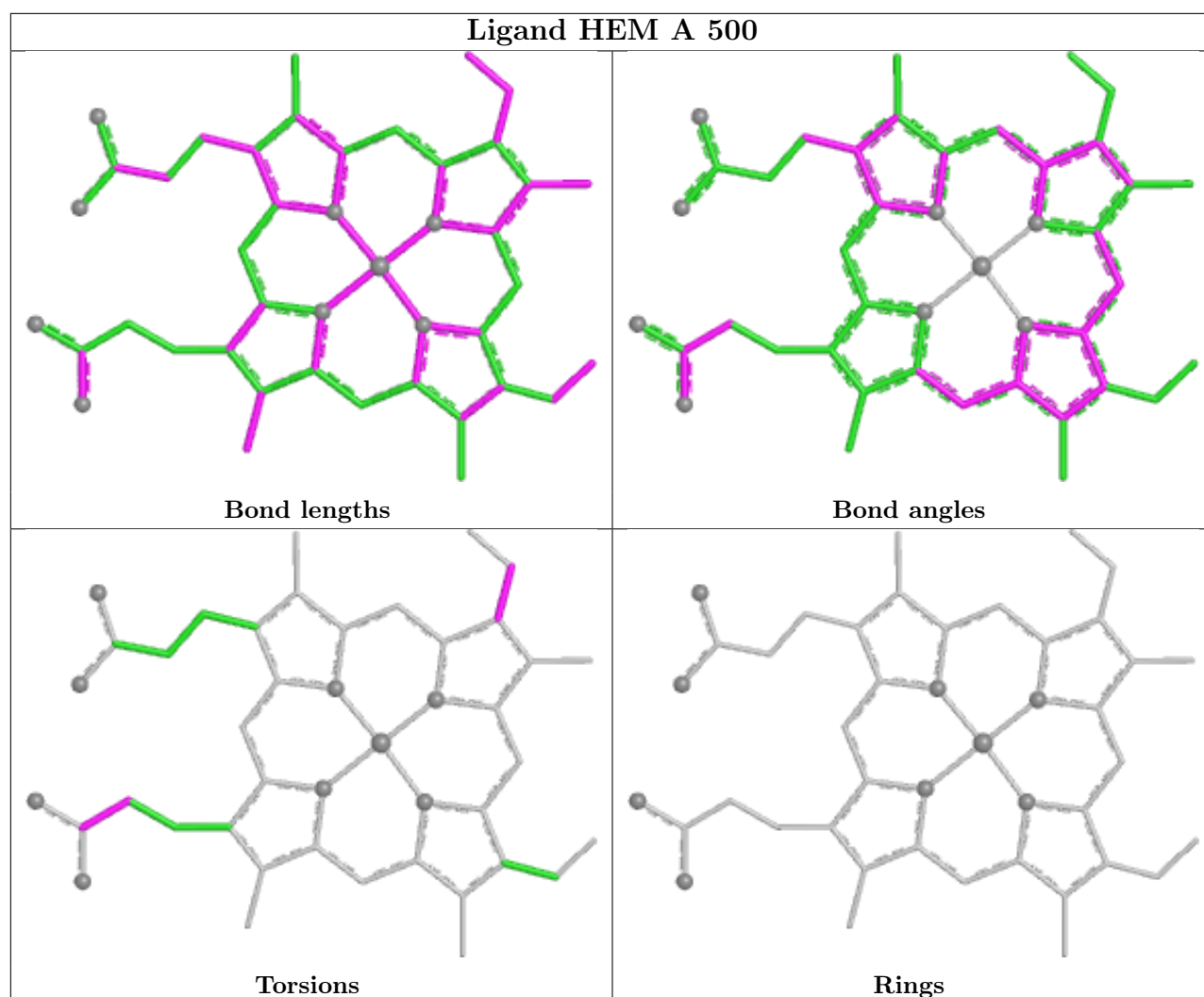
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	500	HEM	2	0
2	B	500	HEM	1	0
2	A	500	HEM	2	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	464/476 (97%)	-0.11	2 (0%) 88 84	15, 48, 81, 107	1 (0%)
1	B	464/476 (97%)	-0.00	1 (0%) 91 88	24, 53, 86, 136	0
1	C	464/476 (97%)	-0.13	1 (0%) 91 88	22, 49, 81, 120	0
1	D	464/476 (97%)	-0.11	0 100 100	23, 50, 79, 134	0
All	All	1856/1904 (97%)	-0.09	4 (0%) 91 88	15, 50, 82, 136	1 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	370	LEU	4.1
1	B	236	GLN	2.3
1	C	388	GLY	2.2
1	A	133	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

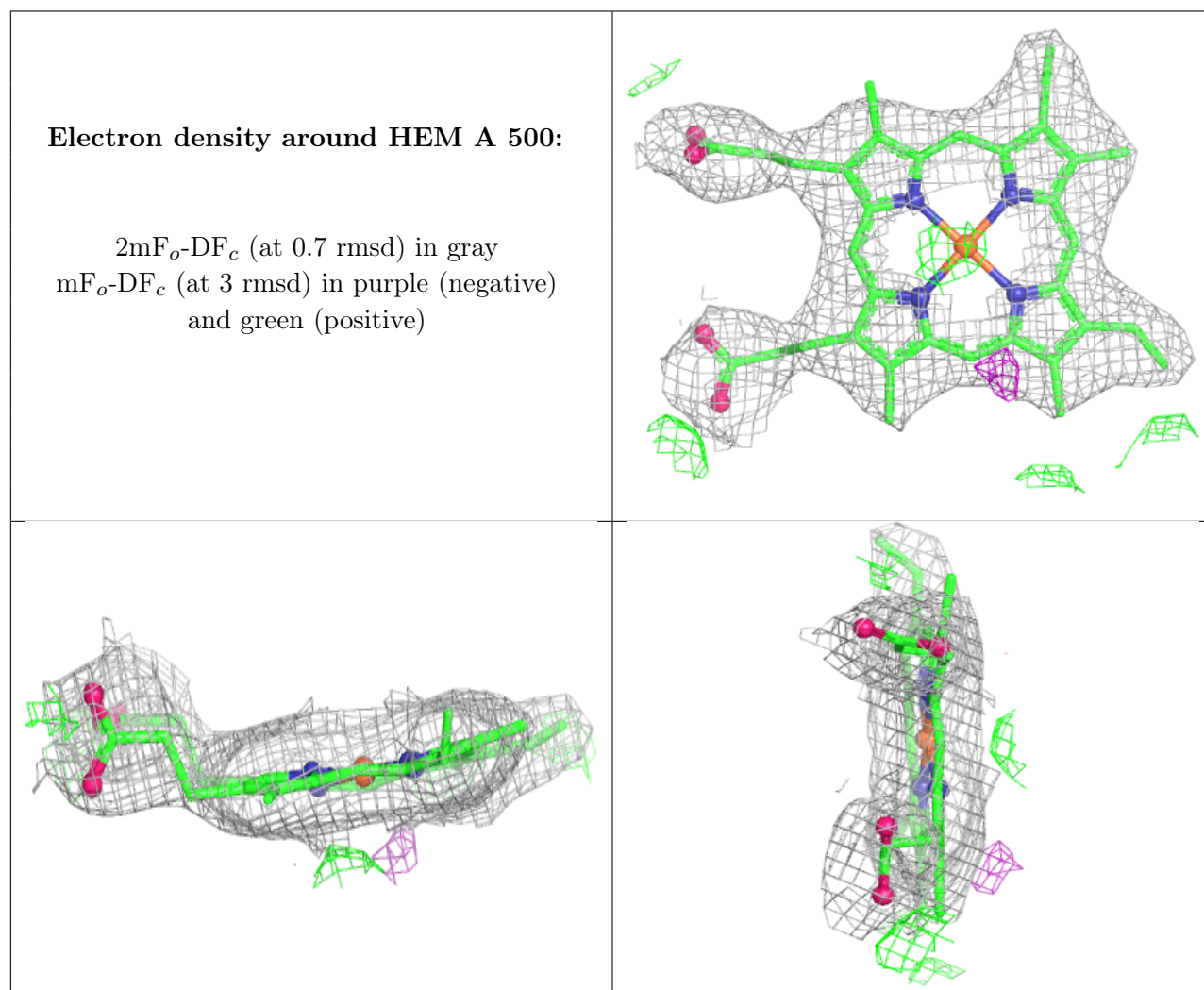
There are no oligosaccharides in this entry.

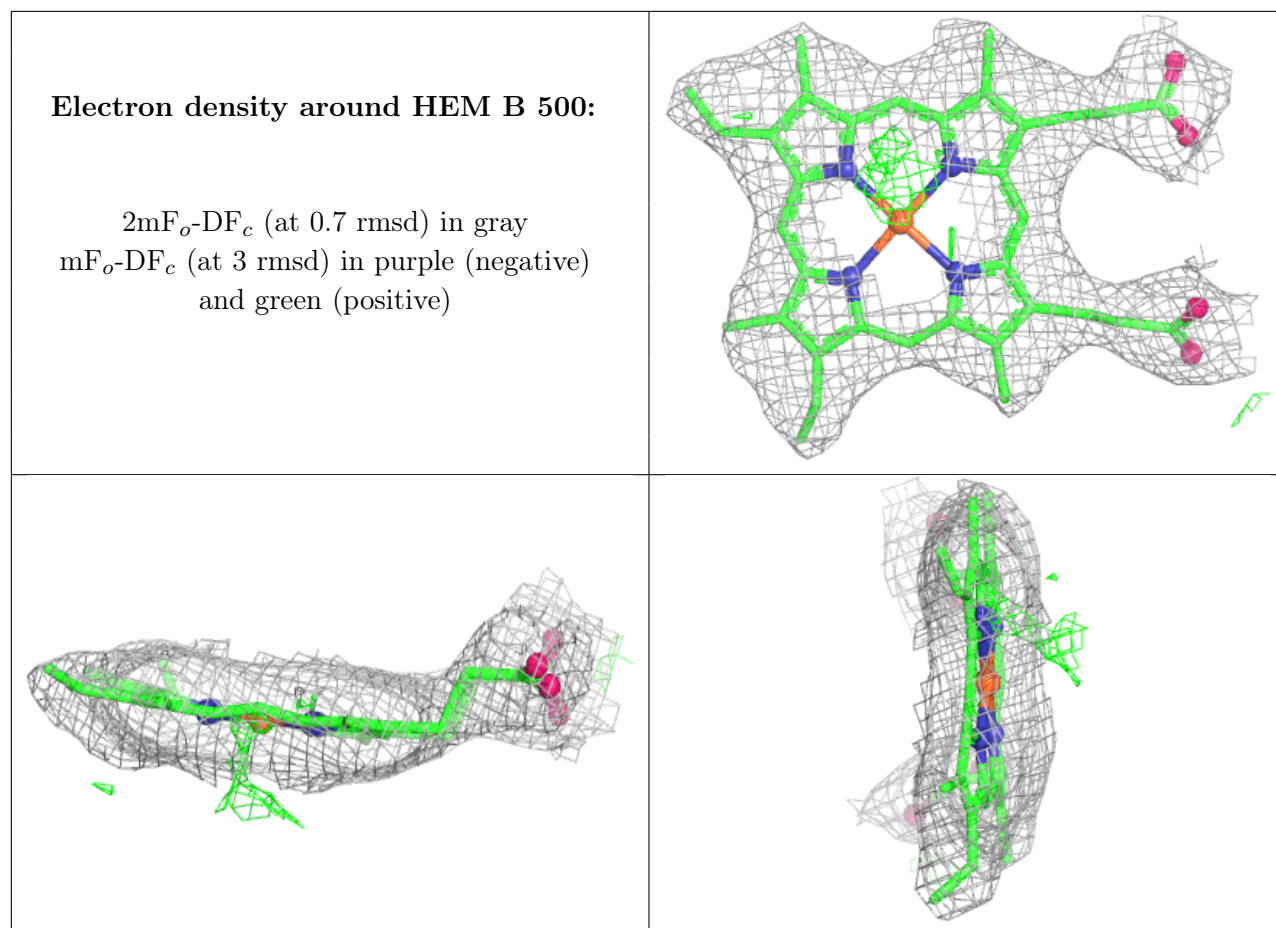
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	HEM	A	500	43/43	0.96	0.10	48,48,48,48	0
2	HEM	B	500	43/43	0.97	0.10	48,48,48,48	0
2	HEM	C	500	43/43	0.97	0.09	48,48,48,48	0
2	HEM	D	500	43/43	0.97	0.09	48,48,48,48	0

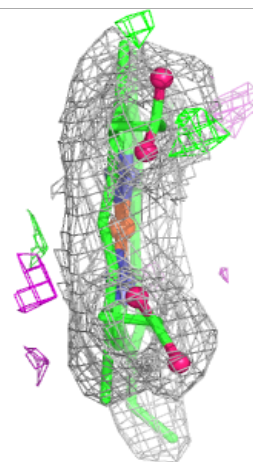
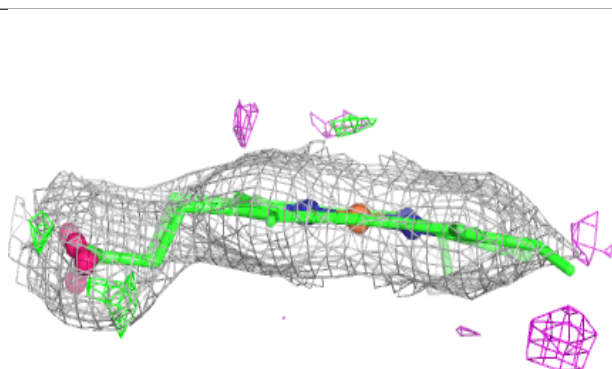
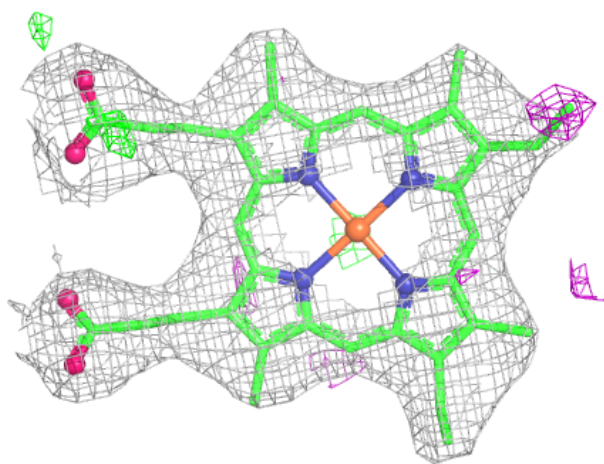
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

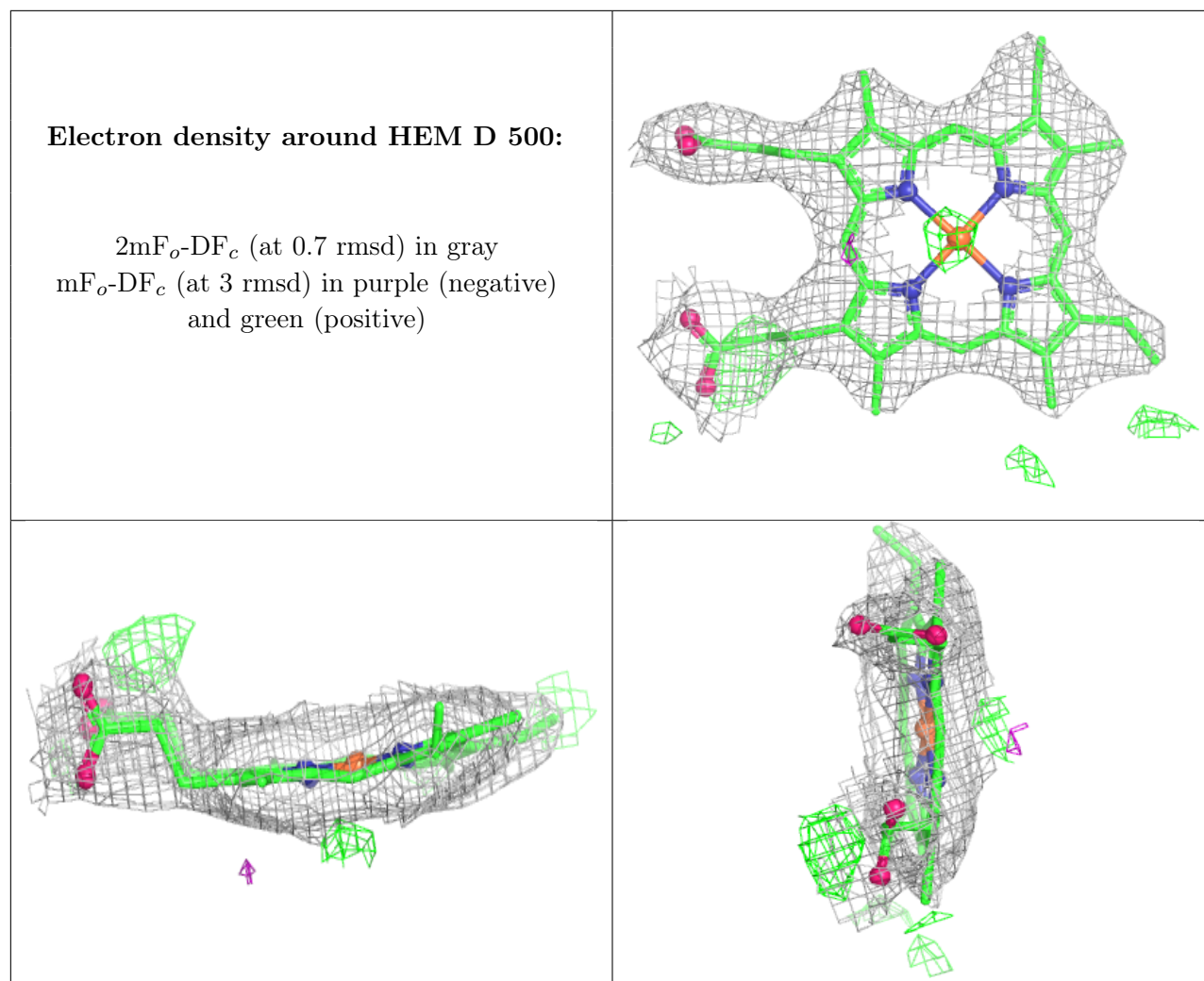




Electron density around HEM C 500:

$2mF_o-DF_c$ (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.