



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 11:05 pm BST

PDB ID : 3UA5  
Title : Crystal Structure of P450 2B6 (Y226H/K262R) in complex with two molecules of Amlodipine  
Authors : Shah, M.B.; Stout, C.D.; Halpert, J.R.  
Deposited on : 2011-10-21  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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 : 2.11  
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) : 2.11

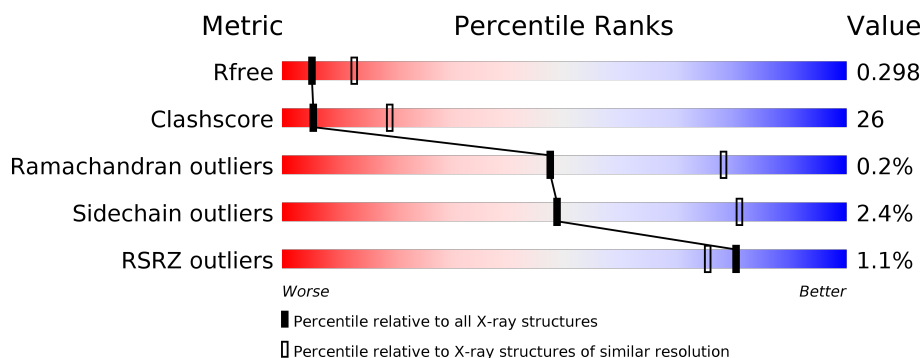
# 1 Overall quality at a glance

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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	476	<div> <div>%</div> <div> <div></div> <div>64%</div> <div>31%</div> <div>••</div> </div> </div>
1	B	476	<div> <div>%</div> <div> <div></div> <div>65%</div> <div>30%</div> <div>••</div> </div> </div>

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
2	HEM	A	500	-	-	X	-
3	06X	A	501	-	-	X	-
3	06X	A	502	-	-	X	X
3	06X	B	501	-	-	X	-
3	06X	B	502	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7660 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 2B6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	1	0
			3700	2394	630	659	17			
1	B	462	Total	C	N	O	S	0	0	0
			3684	2388	630	650	16			

There are 30 discrepancies between the modelled and reference sequences:

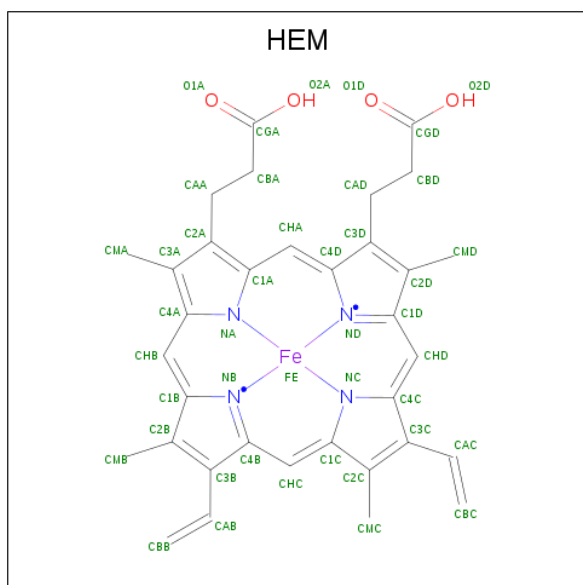
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	GLU	ENGINEERED MUTATION	UNP P20813
A	22	LYS	ARG	ENGINEERED MUTATION	UNP P20813
A	23	LYS	HIS	ENGINEERED MUTATION	UNP P20813
A	24	THR	PRO	ENGINEERED MUTATION	UNP P20813
A	25	SER	ASN	ENGINEERED MUTATION	UNP P20813
A	26	SER	THR	ENGINEERED MUTATION	UNP P20813
A	27	LYS	HIS	ENGINEERED MUTATION	UNP P20813
A	28	GLY	ASP	ENGINEERED MUTATION	UNP P20813
A	29	LYS	ARG	ENGINEERED MUTATION	UNP P20813
A	226	HIS	TYR	ENGINEERED MUTATION	UNP P20813
A	262	ARG	LYS	ENGINEERED MUTATION	UNP P20813
A	492	HIS	-	EXPRESSION TAG	UNP P20813
A	493	HIS	-	EXPRESSION TAG	UNP P20813
A	494	HIS	-	EXPRESSION TAG	UNP P20813
A	495	HIS	-	EXPRESSION TAG	UNP P20813
B	2	ALA	GLU	ENGINEERED MUTATION	UNP P20813
B	22	LYS	ARG	ENGINEERED MUTATION	UNP P20813
B	23	LYS	HIS	ENGINEERED MUTATION	UNP P20813
B	24	THR	PRO	ENGINEERED MUTATION	UNP P20813
B	25	SER	ASN	ENGINEERED MUTATION	UNP P20813
B	26	SER	THR	ENGINEERED MUTATION	UNP P20813
B	27	LYS	HIS	ENGINEERED MUTATION	UNP P20813
B	28	GLY	ASP	ENGINEERED MUTATION	UNP P20813
B	29	LYS	ARG	ENGINEERED MUTATION	UNP P20813
B	226	HIS	TYR	ENGINEERED MUTATION	UNP P20813

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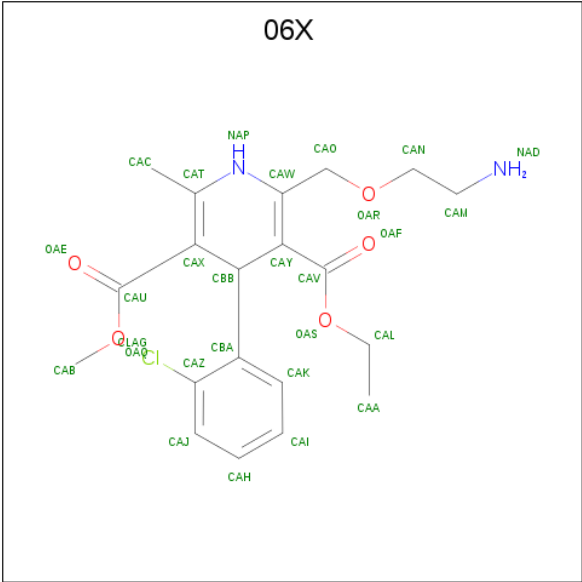
Chain	Residue	Modelled	Actual	Comment	Reference
B	262	ARG	LYS	ENGINEERED MUTATION	UNP P20813
B	492	HIS	-	EXPRESSION TAG	UNP P20813
B	493	HIS	-	EXPRESSION TAG	UNP P20813
B	494	HIS	-	EXPRESSION TAG	UNP P20813
B	495	HIS	-	EXPRESSION TAG	UNP P20813

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



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

- Molecule 3 is Amlodipine (three-letter code: 06X) (formula:  $\text{C}_{20}\text{H}_{25}\text{ClN}_2\text{O}_5$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			28	20	1	2	5		
3	A	1	Total	C	Cl	N	O	0	0
			28	20	1	2	5		
3	B	1	Total	C	Cl	N	O	0	0
			28	20	1	2	5		
3	B	1	Total	C	Cl	N	O	0	0
			28	20	1	2	5		

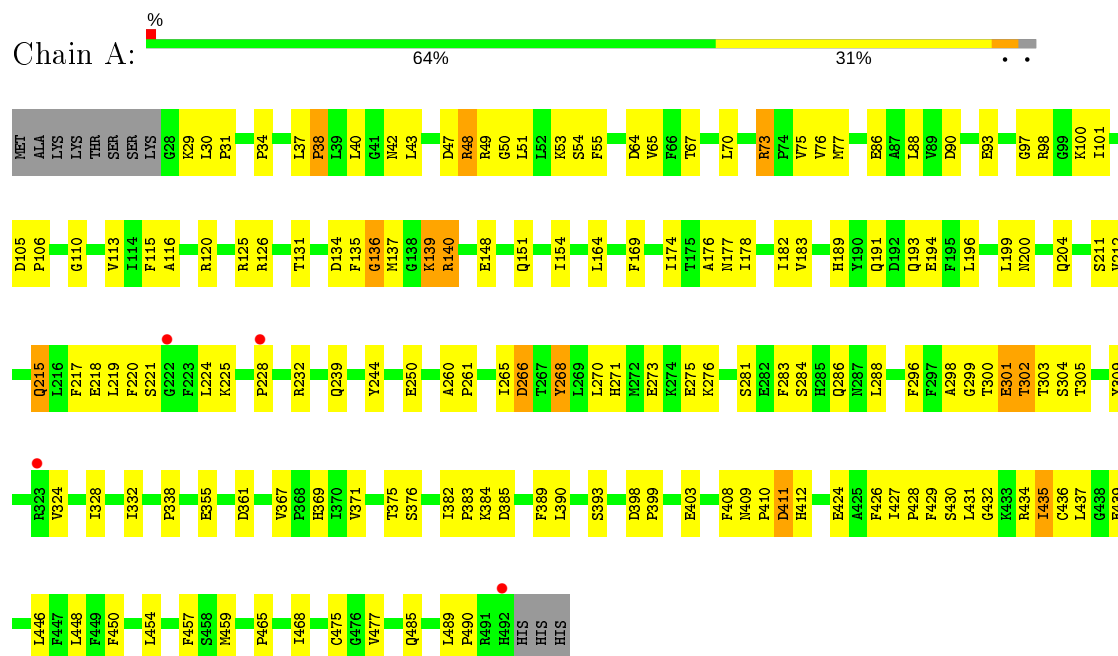
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	40	Total	O	0	0
			40	40		
4	B	38	Total	O	0	0
			38	38		

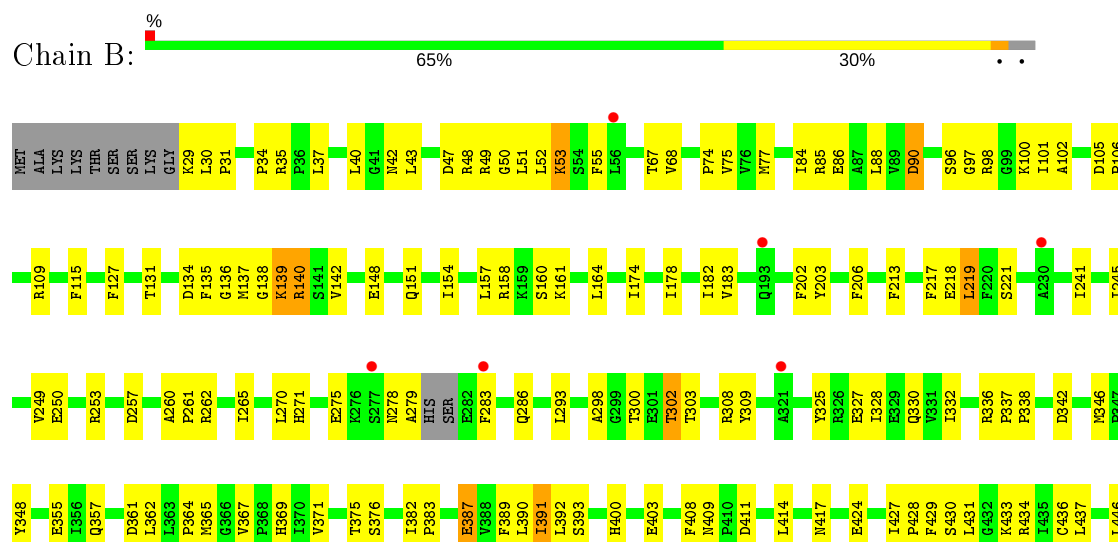
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 2B6



#### • Molecule 1: Cytochrome P450 2B6







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.00 Å 78.30 Å 247.34 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.45 – 2.80 82.45 – 2.80	Depositor EDS
% Data completeness (in resolution range)	90.4 (82.45-2.80) 90.4 (82.45-2.80)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 2.82 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.242 , 0.294 0.246 , 0.298	Depositor DCC
$R_{free}$ test set	1304 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.8	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7660	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, 06X

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	0.94	2/3801 (0.1%)	0.81	2/5150 (0.0%)
1	B	0.90	0/3781	0.83	3/5122 (0.1%)
All	All	0.92	2/7582 (0.0%)	0.82	5/10272 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	PRO	N-CD	-7.75	1.37	1.47
1	A	250	GLU	CG-CD	5.13	1.59	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	219	LEU	CA-CB-CG	-5.96	101.59	115.30
1	B	391	ILE	N-CA-C	-5.70	95.61	111.00
1	A	64	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	A	266	ASP	CB-CG-OD1	5.05	122.85	118.30
1	B	392	LEU	CB-CG-CD2	-5.04	102.43	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	48	ARG	Sidechain
1	A	73	ARG	Sidechain

## 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	3700	0	3635	179	0
1	B	3684	0	3623	150	0
2	A	43	0	30	22	0
2	B	43	0	30	20	0
3	A	56	0	49	37	0
3	B	56	0	49	37	0
4	A	40	0	0	9	0
4	B	38	0	0	5	0
All	All	7660	0	7416	388	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 26.

All (388) 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:A:502:06X:CAI	3:A:502:06X:H8	1.43	1.47
3:B:502:06X:CAI	3:B:502:06X:H8	1.70	1.22
1:A:302:THR:HG22	1:A:303:THR:N	1.56	1.13
1:A:302:THR:HG23	2:A:500:HEM:HAB	1.27	1.13
3:A:502:06X:CAI	3:A:502:06X:CAA	2.30	1.09
1:A:477:VAL:HG23	1:A:477:VAL:O	1.51	1.08
1:A:302:THR:HG22	1:A:303:THR:H	0.93	1.07
1:B:29:LYS:HG3	1:B:30:LEU:H	1.16	1.06
1:A:100:LYS:HG3	1:A:105[A]:ASP:OD2	1.57	1.05
1:A:212:VAL:HG23	4:A:631:HOH:O	1.65	0.96
2:B:500:HEM:HBB2	2:B:500:HEM:CMB	1.94	0.96
1:B:30:LEU:HG	1:B:31:PRO:HD2	1.49	0.94
3:A:501:06X:H17	3:A:501:06X:OAF	1.69	0.93
1:B:302:THR:HG23	2:B:500:HEM:CAB	1.98	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:500:HEM:HBB2	2:B:500:HEM:HMB1	1.48	0.91
3:A:502:06X:H17	3:A:502:06X:OAF	1.68	0.91
1:A:302:THR:CG2	1:A:303:THR:N	2.29	0.91
1:B:302:THR:HG22	1:B:303:THR:N	1.86	0.90
1:B:461:SER:OG	1:B:462:PRO:HD2	1.70	0.89
1:A:116:ALA:O	1:A:434:ARG:NH2	2.06	0.89
1:B:302:THR:HG21	2:B:500:HEM:HHC	1.53	0.88
3:B:501:06X:OAF	3:B:501:06X:H17	1.70	0.87
3:A:502:06X:H3	3:A:502:06X:H8	1.53	0.87
1:A:93:GLU:HB3	4:A:601:HOH:O	1.72	0.87
1:B:365:MET:HG2	1:B:391:ILE:HD12	1.56	0.87
1:B:409:ASN:OD1	1:B:411:ASP:HB2	1.72	0.87
1:A:302:THR:HG23	2:A:500:HEM:CAB	2.06	0.86
1:A:55:PHE:HE1	1:A:77:MET:HE3	1.38	0.85
1:A:218:GLU:C	1:A:219:LEU:HD23	1.97	0.84
1:A:302:THR:CG2	2:A:500:HEM:HAB	2.07	0.84
1:A:164:LEU:HD22	1:A:485:GLN:HB3	1.61	0.82
3:B:502:06X:OAS	3:B:502:06X:CBA	2.26	0.82
1:A:429:PHE:HB2	4:A:608:HOH:O	1.79	0.81
1:A:477:VAL:CG2	1:A:477:VAL:O	2.22	0.81
3:A:502:06X:CAH	3:A:502:06X:CAA	2.59	0.80
3:B:502:06X:CAA	3:B:502:06X:CAI	2.56	0.80
3:A:502:06X:CAK	3:A:502:06X:H8	2.09	0.80
1:A:224:LEU:O	1:A:224:LEU:HD12	1.81	0.80
3:A:501:06X:OAS	3:A:501:06X:CBA	2.30	0.80
3:B:502:06X:H3	3:B:502:06X:H8	1.63	0.80
1:B:434:ARG:O	2:B:500:HEM:HBA2	1.82	0.80
3:A:502:06X:CAH	3:A:502:06X:H8	2.13	0.79
1:A:389:PHE:HZ	3:A:502:06X:H3	1.48	0.79
3:A:502:06X:CBA	3:A:502:06X:OAS	2.30	0.79
1:B:100:LYS:HG2	1:B:105:ASP:OD2	1.82	0.79
1:A:302:THR:CG2	1:A:303:THR:H	1.77	0.79
1:A:37:LEU:HB3	1:A:38:PRO:CD	2.13	0.78
1:B:29:LYS:HG3	1:B:30:LEU:N	1.98	0.78
1:B:302:THR:HG21	2:B:500:HEM:CHC	2.14	0.78
3:B:502:06X:CBA	3:B:502:06X:OAE	2.31	0.78
2:B:500:HEM:CBB	2:B:500:HEM:HMB1	2.14	0.77
3:B:501:06X:CBA	3:B:501:06X:OAS	2.30	0.77
1:A:169:PHE:HD2	4:A:613:HOH:O	1.67	0.77
3:B:501:06X:CBA	3:B:501:06X:OAE	2.30	0.77
1:B:164:LEU:HD22	1:B:485:GLN:HB3	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:502:06X:OAE	3:A:502:06X:CBA	2.30	0.77
1:A:37:LEU:HB3	1:A:38:PRO:HD2	1.69	0.75
3:A:501:06X:CBA	3:A:501:06X:OAE	2.30	0.75
3:B:502:06X:OAS	3:B:502:06X:CAK	2.35	0.75
1:A:134:ASP:O	1:A:137:MET:HB3	1.87	0.74
3:B:502:06X:OAF	3:B:502:06X:H17	1.87	0.74
1:A:435:ILE:O	1:A:435:ILE:CG2	2.34	0.74
1:B:49:ARG:HG3	1:B:49:ARG:O	1.88	0.73
1:B:461:SER:OG	1:B:462:PRO:CD	2.36	0.73
1:A:189:HIS:HB3	4:A:615:HOH:O	1.89	0.72
1:B:328:ILE:HG23	1:B:332:ILE:HD12	1.72	0.72
1:B:361:ASP:OD2	1:B:393:SER:HB2	1.90	0.71
1:A:100:LYS:CG	1:A:105[A]:ASP:OD2	2.37	0.71
1:A:409:ASN:OD1	1:A:411:ASP:HB2	1.91	0.71
1:B:142:VAL:HG23	4:B:605:HOH:O	1.91	0.70
1:A:361:ASP:OD2	1:A:393:SER:HB2	1.91	0.70
1:A:218:GLU:O	1:A:219:LEU:HD23	1.90	0.70
3:A:501:06X:CAC	3:A:501:06X:OAQ	2.37	0.70
1:A:34:PRO:HG2	1:A:42:ASN:ND2	2.07	0.70
3:B:501:06X:CAC	3:B:501:06X:OAQ	2.37	0.70
1:B:84:ILE:HD11	1:B:391:ILE:O	1.91	0.70
3:A:502:06X:OAQ	3:A:502:06X:CAC	2.37	0.70
3:B:502:06X:CAC	3:B:502:06X:OAQ	2.37	0.70
1:A:302:THR:HG21	2:A:500:HEM:HHC	1.75	0.69
1:A:219:LEU:HD23	1:A:219:LEU:N	2.03	0.68
1:A:232:ARG:HG3	1:B:260:ALA:HB1	1.75	0.68
1:B:434:ARG:O	2:B:500:HEM:CBA	2.42	0.68
1:B:75:VAL:HG22	1:B:387:GLU:HB3	1.75	0.68
1:A:219:LEU:HD21	3:A:502:06X:H5	1.76	0.68
1:A:273:GLU:O	1:A:276:LYS:HG2	1.94	0.68
1:A:302:THR:CG2	2:A:500:HEM:HHC	2.24	0.68
1:B:302:THR:CG2	1:B:303:THR:N	2.56	0.68
3:A:502:06X:CAH	3:A:502:06X:H9	2.24	0.67
3:B:501:06X:OAE	3:B:501:06X:CAK	2.44	0.66
1:A:55:PHE:CE1	1:A:77:MET:HE3	2.26	0.66
1:A:50:GLY:O	1:A:53:LYS:HB3	1.94	0.66
3:B:502:06X:CAH	3:B:502:06X:H8	2.23	0.65
1:A:424:GLU:HG3	4:A:635:HOH:O	1.96	0.65
1:B:43:LEU:HD21	1:B:219:LEU:HD13	1.79	0.64
2:B:500:HEM:HBC2	2:B:500:HEM:HMC2	1.79	0.64
1:B:298:ALA:O	3:B:501:06X:H20	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:PHE:HB3	4:A:637:HOH:O	1.98	0.64
1:A:126:ARG:HB2	4:A:610:HOH:O	1.98	0.64
1:B:47:ASP:OD1	1:B:48:ARG:N	2.31	0.64
1:A:281:SER:OG	1:A:284:SER:HB2	1.97	0.64
1:B:389:PHE:HZ	3:B:502:06X:H3	1.63	0.63
1:B:465:PRO:HA	1:B:468:ILE:HD12	1.81	0.63
1:A:430:SER:CB	2:A:500:HEM:O2A	2.46	0.63
1:A:98:ARG:NH1	1:A:367:VAL:HG12	2.14	0.62
1:B:283:PHE:O	1:B:286:GLN:HB2	2.00	0.62
1:B:429:PHE:O	1:B:430:SER:HB3	1.99	0.62
1:A:465:PRO:HA	1:A:468:ILE:HD12	1.80	0.62
1:A:435:ILE:O	1:A:435:ILE:HG22	1.99	0.62
1:A:239:GLN:HB3	1:B:138:GLY:O	2.00	0.62
1:A:174:ILE:O	1:A:178:ILE:HG12	1.99	0.61
1:B:355:GLU:HG3	1:B:408:PHE:CE1	2.36	0.61
1:A:125:ARG:HH22	1:A:435:ILE:HG22	1.65	0.61
1:A:224:LEU:O	1:A:224:LEU:CD1	2.48	0.61
1:B:40:LEU:O	1:B:43:LEU:HB2	2.01	0.61
1:A:169:PHE:CD2	4:A:613:HOH:O	2.45	0.60
3:B:502:06X:OAF	3:B:502:06X:CAO	2.49	0.60
1:B:430:SER:OG	1:B:431:LEU:N	2.34	0.60
1:A:135:PHE:C	1:A:137:MET:H	2.05	0.60
1:A:211:SER:O	1:A:215:GLN:HG2	2.00	0.60
1:A:211:SER:O	1:A:215:GLN:CG	2.51	0.59
1:B:29:LYS:CG	1:B:30:LEU:H	1.95	0.59
1:B:140:ARG:HH12	1:B:148:GLU:CD	2.06	0.59
1:B:427:ILE:O	1:B:427:ILE:HG13	2.00	0.59
1:A:55:PHE:HE1	1:A:77:MET:CE	2.15	0.59
1:A:261:PRO:HG3	1:A:270:LEU:HD11	1.84	0.59
1:B:88:LEU:HD11	1:B:390:LEU:HG	1.85	0.59
1:B:102:ALA:N	1:B:218:GLU:OE2	2.36	0.58
1:B:302:THR:HG22	1:B:303:THR:H	1.65	0.58
1:B:30:LEU:HG	1:B:31:PRO:CD	2.28	0.58
3:B:501:06X:CAU	3:B:501:06X:CAK	2.79	0.58
1:A:436:CYS:HB2	2:A:500:HEM:C4A	2.39	0.58
1:B:52:LEU:HD22	1:B:364:PRO:CB	2.33	0.58
1:A:298:ALA:O	3:A:501:06X:H20	2.04	0.57
1:B:446:LEU:O	1:B:450:PHE:HB2	2.04	0.57
1:A:191:GLN:O	1:A:193:GLN:NE2	2.32	0.57
1:A:301:GLU:CA	1:A:301:GLU:OE1	2.49	0.57
1:B:115:PHE:HE1	3:B:501:06X:H7	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:VAL:HG12	2:A:500:HEM:HBD2	1.85	0.57
1:B:98:ARG:NH1	1:B:367:VAL:CG1	2.68	0.57
1:B:55:PHE:HE1	1:B:77:MET:HE3	1.69	0.57
1:A:40:LEU:O	1:A:43:LEU:HB2	2.05	0.57
3:A:502:06X:CAK	3:A:502:06X:OAS	2.53	0.57
1:B:183:VAL:O	1:B:265:ILE:HG12	2.05	0.57
1:B:34:PRO:HG2	1:B:42:ASN:ND2	2.20	0.56
1:B:400:HIS:HB3	4:B:620:HOH:O	2.04	0.56
1:B:151:GLN:O	1:B:154:ILE:HG13	2.06	0.56
1:B:355:GLU:HG3	1:B:408:PHE:CD1	2.40	0.56
2:B:500:HEM:CMC	2:B:500:HEM:HBC2	2.35	0.56
3:B:502:06X:CAL	3:B:502:06X:CAK	2.83	0.56
1:B:34:PRO:HB2	1:B:42:ASN:ND2	2.21	0.56
1:A:140:ARG:HH12	1:A:148:GLU:CD	2.09	0.56
3:A:501:06X:OAE	3:A:501:06X:CAK	2.54	0.55
1:A:49:ARG:O	1:A:49:ARG:HG3	2.05	0.55
1:B:157:LEU:O	1:B:160:SER:HB3	2.05	0.55
1:B:245:ILE:O	1:B:249:VAL:HG23	2.06	0.55
1:B:389:PHE:CZ	3:B:502:06X:H3	2.40	0.55
1:B:361:ASP:HB3	1:B:479:LYS:HD2	1.87	0.55
1:A:224:LEU:O	1:A:224:LEU:CG	2.54	0.55
1:A:301:GLU:OE1	1:A:305:THR:OG1	2.23	0.55
1:B:302:THR:HG23	2:B:500:HEM:HAB	1.87	0.54
1:B:302:THR:HA	1:B:362:LEU:HD21	1.89	0.54
1:B:302:THR:CG2	2:B:500:HEM:CAB	2.81	0.54
1:A:169:PHE:CE2	1:A:196:LEU:HD22	2.42	0.54
1:B:51:LEU:O	1:B:52:LEU:C	2.44	0.54
1:A:88:LEU:HD11	1:A:390:LEU:HG	1.90	0.54
1:A:125:ARG:NH2	1:A:435:ILE:HG22	2.23	0.54
1:A:55:PHE:CE1	1:A:77:MET:CE	2.89	0.54
1:A:220:PHE:O	1:A:224:LEU:HB3	2.08	0.53
1:B:101:ILE:HG21	3:B:501:06X:H2	1.89	0.53
1:B:98:ARG:NH1	1:B:367:VAL:HG12	2.23	0.53
1:A:300:THR:O	1:A:301:GLU:CB	2.56	0.53
1:B:261:PRO:HG3	1:B:270:LEU:HD11	1.91	0.53
1:A:228:PRO:HB2	1:B:257:ASP:HB2	1.90	0.53
1:A:232:ARG:HD2	1:B:262:ARG:CG	2.38	0.53
1:B:206:PHE:CZ	1:B:300:THR:HB	2.44	0.53
1:A:260:ALA:N	1:A:261:PRO:HD3	2.24	0.53
1:A:431:LEU:HA	1:A:435:ILE:HG13	1.90	0.53
1:B:260:ALA:N	1:B:261:PRO:HD3	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:CYS:HB2	2:A:500:HEM:NA	2.23	0.53
1:B:357:GLN:NE2	1:B:429:PHE:CZ	2.77	0.53
1:A:232:ARG:HG3	1:B:260:ALA:CB	2.37	0.52
1:A:268:TYR:CD1	1:A:288:LEU:HD13	2.44	0.52
1:A:475:CYS:SG	1:A:475:CYS:O	2.67	0.52
3:A:501:06X:OAF	3:A:501:06X:CAO	2.47	0.52
1:A:101:ILE:HG22	1:A:101:ILE:O	2.10	0.52
1:A:151:GLN:O	1:A:154:ILE:HG13	2.10	0.52
3:B:502:06X:OAQ	3:B:502:06X:H15	2.10	0.52
1:A:136:GLY:HA2	1:A:139:LYS:O	2.10	0.52
1:B:375:THR:HG22	1:B:376:SER:N	2.22	0.52
1:B:100:LYS:CG	1:B:105:ASP:OD2	2.57	0.52
1:A:135:PHE:O	1:A:137:MET:N	2.43	0.52
1:B:434:ARG:HB3	2:B:500:HEM:O1A	2.10	0.51
1:A:430:SER:OG	1:A:431:LEU:N	2.43	0.51
1:A:426:PHE:CZ	1:A:428:PRO:HG3	2.46	0.51
1:B:302:THR:CG2	2:B:500:HEM:HHC	2.35	0.51
1:A:283:PHE:O	1:A:286:GLN:HB2	2.11	0.51
3:A:501:06X:OAQ	3:A:501:06X:H15	2.11	0.51
3:A:502:06X:CAK	3:A:502:06X:OAE	2.59	0.51
1:B:434:ARG:O	2:B:500:HEM:CGA	2.59	0.51
3:A:501:06X:OAS	3:A:501:06X:CAK	2.58	0.50
1:B:454:LEU:HD21	1:B:459:MET:CE	2.41	0.50
1:A:271:HIS:O	1:A:275:GLU:HB2	2.11	0.50
1:B:98:ARG:HH11	1:B:367:VAL:HG12	1.76	0.50
1:A:50:GLY:O	1:A:53:LYS:N	2.45	0.50
1:A:261:PRO:HG3	1:A:270:LEU:CD1	2.41	0.50
1:A:232:ARG:HD2	1:B:262:ARG:HG2	1.94	0.50
1:B:86:GLU:O	1:B:90:ASP:HB2	2.11	0.50
1:A:301:GLU:OE1	1:A:301:GLU:O	2.30	0.49
1:B:174:ILE:O	1:B:178:ILE:HG12	2.11	0.49
1:B:475:CYS:O	1:B:475:CYS:SG	2.70	0.49
1:A:296:PHE:O	1:A:300:THR:OG1	2.29	0.49
1:B:391:ILE:HD13	1:B:391:ILE:N	2.28	0.49
1:B:454:LEU:HD21	1:B:459:MET:HE3	1.94	0.49
1:B:457:PHE:O	1:B:491:ARG:NH1	2.45	0.49
1:A:135:PHE:CD2	1:A:136:GLY:N	2.80	0.49
3:A:502:06X:H15	3:A:502:06X:OAQ	2.11	0.49
1:B:158:ARG:O	1:B:161:LYS:N	2.43	0.49
1:B:241:ILE:HG21	1:B:293:LEU:HD11	1.95	0.49
3:B:501:06X:CAV	3:B:501:06X:H18	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:PRO:CB	1:B:257:ASP:HB2	2.42	0.49
1:A:390:LEU:HD22	1:A:390:LEU:N	2.27	0.49
1:A:218:GLU:HG3	3:A:502:06X:CLAG	2.50	0.49
1:B:31:PRO:HB2	1:B:67:THR:OG1	2.13	0.49
1:A:355:GLU:HG3	1:A:408:PHE:CE1	2.47	0.49
1:A:410:PRO:O	1:A:412:HIS:N	2.45	0.49
1:A:273:GLU:HA	1:A:276:LYS:HG2	1.95	0.49
1:A:328:ILE:HG23	1:A:332:ILE:HD12	1.94	0.49
1:B:375:THR:CG2	1:B:376:SER:N	2.76	0.48
1:A:427:ILE:N	1:A:428:PRO:CD	2.76	0.48
1:A:429:PHE:CE2	1:A:439:GLU:HG3	2.48	0.48
1:B:115:PHE:CE1	3:B:501:06X:H7	2.48	0.48
1:B:52:LEU:HD22	1:B:364:PRO:HB3	1.95	0.48
1:A:169:PHE:CE2	1:A:196:LEU:CD2	2.96	0.48
3:A:501:06X:OAQ	3:A:501:06X:H14	2.14	0.48
3:A:502:06X:H14	3:A:502:06X:OAQ	2.14	0.48
1:A:113:VAL:CG1	2:A:500:HEM:HBD2	2.43	0.48
1:A:100:LYS:O	1:A:101:ILE:HG13	2.14	0.48
1:A:70:LEU:HD12	1:A:75:VAL:HG21	1.96	0.48
1:B:75:VAL:O	1:B:77:MET:HE2	2.14	0.48
1:B:278:ASN:O	1:B:279:ALA:HB3	2.14	0.47
3:B:501:06X:OAF	3:B:501:06X:H18	2.14	0.47
1:A:355:GLU:HG2	1:A:409:ASN:C	2.35	0.47
3:B:501:06X:H15	3:B:501:06X:OAQ	2.11	0.47
1:B:437:LEU:HB3	2:B:500:HEM:HMD2	1.95	0.47
1:A:125:ARG:NH1	2:A:500:HEM:O1D	2.45	0.47
1:A:183:VAL:O	1:A:265:ILE:HG12	2.14	0.47
1:B:261:PRO:HG3	1:B:270:LEU:CD1	2.45	0.47
1:A:115:PHE:CE1	3:A:501:06X:H7	2.50	0.47
1:A:178:ILE:O	1:A:182:ILE:HG13	2.14	0.47
1:A:332:ILE:HD13	1:A:338:PRO:HB3	1.96	0.47
1:A:367:VAL:O	1:A:369:HIS:HD2	1.98	0.47
1:B:330:GLN:HA	1:B:330:GLN:OE1	2.15	0.47
1:A:151:GLN:HA	1:A:154:ILE:HG12	1.97	0.47
1:B:362:LEU:HD12	4:B:619:HOH:O	2.15	0.47
1:B:348:TYR:HD1	1:B:414:LEU:HD11	1.80	0.46
1:A:51:LEU:HD22	3:A:502:06X:H18	1.95	0.46
1:A:73:ARG:HB3	1:A:73:ARG:HH21	1.79	0.46
1:A:200:ASN:O	1:A:204:GLN:HB2	2.15	0.46
1:A:266:ASP:O	1:A:270:LEU:HG	2.15	0.46
1:A:437:LEU:HB3	2:A:500:HEM:HMD2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:HIS:O	1:B:275:GLU:HB2	2.16	0.46
1:B:332:ILE:HD13	1:B:338:PRO:HB3	1.97	0.46
1:A:97:GLY:O	1:A:369:HIS:HA	2.16	0.46
3:B:501:06X:H14	3:B:501:06X:OAQ	2.14	0.46
1:A:302:THR:CG2	2:A:500:HEM:CHC	2.92	0.46
1:B:96:SER:OG	1:B:433:LYS:HD2	2.16	0.46
1:A:437:LEU:HB3	2:A:500:HEM:CMD	2.46	0.46
3:B:502:06X:CAK	3:B:502:06X:CAV	2.91	0.46
1:B:68:VAL:HB	1:B:77:MET:HE3	1.97	0.46
1:A:389:PHE:HZ	3:A:502:06X:CAI	2.25	0.46
1:A:457:PHE:HA	1:A:489:LEU:O	2.15	0.46
1:B:308:ARG:HD3	4:B:606:HOH:O	2.15	0.46
1:A:302:THR:HG21	2:A:500:HEM:CHC	2.44	0.45
3:B:502:06X:OAE	3:B:502:06X:CAK	2.64	0.45
1:A:194:GLU:OE2	1:A:244:TYR:CE1	2.69	0.45
1:A:29:LYS:O	1:A:30:LEU:C	2.55	0.45
1:A:302:THR:HG23	2:A:500:HEM:HHC	1.96	0.45
1:A:125:ARG:HH11	2:A:500:HEM:CGD	2.30	0.45
1:A:176:ALA:O	1:A:177:ASN:C	2.52	0.45
1:B:219:LEU:HA	1:B:219:LEU:HD23	1.40	0.45
1:A:98:ARG:HH11	1:A:367:VAL:HG12	1.78	0.45
3:B:501:06X:CAZ	3:B:501:06X:OAS	2.65	0.45
1:B:109:ARG:HB3	1:B:109:ARG:HE	1.58	0.45
1:B:325:TYR:HA	1:B:328:ILE:HD12	1.99	0.45
1:A:131:THR:O	1:A:135:PHE:HB2	2.16	0.45
1:A:199:LEU:HD23	1:A:199:LEU:HA	1.89	0.45
1:A:211:SER:O	1:A:215:GLN:HG3	2.17	0.45
1:B:127:PHE:O	1:B:131:THR:OG1	2.27	0.45
1:B:53:LYS:HA	1:B:53:LYS:HD3	1.74	0.45
1:A:217:PHE:O	1:A:221:SER:HB3	2.17	0.45
1:A:30:LEU:HD23	1:A:67:THR:HG21	1.99	0.45
1:A:47:ASP:OD1	1:A:48:ARG:N	2.49	0.45
1:A:73:ARG:NH2	1:A:73:ARG:HB3	2.32	0.45
1:B:34:PRO:HG2	1:B:42:ASN:CG	2.38	0.45
1:B:131:THR:O	1:B:135:PHE:HB2	2.17	0.44
1:B:217:PHE:O	1:B:221:SER:HB3	2.17	0.44
1:B:457:PHE:C	1:B:491:ARG:NH1	2.71	0.44
3:B:501:06X:CAO	3:B:501:06X:OAF	2.47	0.44
1:A:224:LEU:HG	1:A:224:LEU:O	2.16	0.44
1:B:158:ARG:C	1:B:160:SER:N	2.70	0.44
1:B:427:ILE:N	1:B:428:PRO:CD	2.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:LEU:HD23	1:B:67:THR:HG21	1.99	0.44
1:A:268:TYR:CE1	1:A:288:LEU:HD13	2.51	0.44
3:B:502:06X:H14	3:B:502:06X:OAQ	2.16	0.44
1:A:169:PHE:HE2	1:A:196:LEU:CD2	2.31	0.44
3:A:501:06X:CAU	3:A:501:06X:CAK	2.87	0.44
1:A:221:SER:O	1:A:225:LYS:HG2	2.18	0.44
1:A:48:ARG:HA	1:A:49:ARG:HA	1.68	0.44
1:B:55:PHE:CE1	1:B:77:MET:HE3	2.52	0.44
1:A:301:GLU:OE1	1:A:301:GLU:C	2.55	0.44
1:A:432:GLY:O	1:A:435:ILE:HB	2.18	0.44
1:A:430:SER:OG	2:A:500:HEM:O2A	2.32	0.44
2:B:500:HEM:HBB2	2:B:500:HEM:HMB3	1.90	0.44
1:A:355:GLU:HG3	1:A:408:PHE:CD1	2.53	0.44
1:A:410:PRO:C	1:A:412:HIS:N	2.70	0.44
1:B:429:PHE:O	1:B:430:SER:CB	2.65	0.44
1:A:76:VAL:HG21	1:A:382:ILE:HD13	1.99	0.44
1:B:337:PRO:HA	1:B:338:PRO:HD2	1.78	0.44
1:A:361:ASP:OD2	1:A:393:SER:CB	2.64	0.43
1:A:454:LEU:HD21	1:A:459:MET:HE3	2.00	0.43
3:A:502:06X:CAK	3:A:502:06X:CAA	2.82	0.43
1:B:355:GLU:OE1	1:B:355:GLU:HA	2.17	0.43
3:B:502:06X:CAA	3:B:502:06X:CAH	2.94	0.43
1:A:303:THR:O	1:A:304:SER:C	2.57	0.43
1:B:135:PHE:HA	1:B:139:LYS:HZ1	1.83	0.43
1:B:43:LEU:HA	1:B:43:LEU:HD12	1.90	0.43
1:A:446:LEU:O	1:A:450:PHE:HB2	2.19	0.43
1:A:50:GLY:O	1:A:54:SER:N	2.50	0.43
1:A:382:ILE:HA	1:A:383:PRO:HD3	1.61	0.43
3:B:502:06X:CAK	3:B:502:06X:CAU	2.94	0.43
1:A:86:GLU:O	1:A:90:ASP:HB2	2.18	0.43
1:B:139:LYS:HZ2	1:B:139:LYS:HG2	1.56	0.43
1:B:213:PHE:CD1	1:B:213:PHE:C	2.92	0.43
1:B:327:GLU:OE1	1:B:346:MET:HB3	2.18	0.43
1:B:461:SER:CB	1:B:462:PRO:CD	2.95	0.43
1:B:302:THR:CG2	2:B:500:HEM:HAB	2.48	0.43
1:B:74:PRO:O	1:B:74:PRO:HG2	2.18	0.43
1:B:417:ASN:HA	4:B:636:HOH:O	2.17	0.43
1:B:85:ARG:HH22	1:B:424:GLU:HB3	1.83	0.43
1:A:100:LYS:C	1:A:101:ILE:HG13	2.38	0.43
1:A:37:LEU:CB	1:A:38:PRO:CD	2.79	0.43
1:A:389:PHE:CZ	3:A:502:06X:H3	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:GLY:O	1:B:369:HIS:HA	2.19	0.43
1:A:260:ALA:N	1:A:261:PRO:CD	2.82	0.43
1:B:348:TYR:CD1	1:B:414:LEU:HD11	2.53	0.43
1:B:50:GLY:O	1:B:53:LYS:N	2.52	0.43
1:A:375:THR:HG22	1:A:376:SER:N	2.33	0.42
1:B:139:LYS:H	1:B:139:LYS:HG2	1.46	0.42
1:A:101:ILE:HD13	3:A:501:06X:H8	2.01	0.42
1:A:427:ILE:HG13	1:A:427:ILE:O	2.20	0.42
1:A:324:VAL:O	1:A:328:ILE:HG13	2.20	0.42
1:A:430:SER:HB3	2:A:500:HEM:HBA1	2.02	0.42
1:B:48:ARG:HA	1:B:49:ARG:HA	1.20	0.42
1:A:299:GLY:O	1:A:302:THR:HB	2.20	0.42
1:B:260:ALA:N	1:B:261:PRO:CD	2.82	0.42
1:B:250:GLU:OE1	1:B:253:ARG:HD2	2.20	0.41
2:B:500:HEM:CBC	2:B:500:HEM:HMC2	2.49	0.41
1:B:105:ASP:N	1:B:106:PRO:CD	2.83	0.41
1:B:364:PRO:HD2	1:B:477:VAL:O	2.20	0.41
1:A:31:PRO:HB3	1:A:65:VAL:O	2.21	0.41
1:B:135:PHE:C	1:B:137:MET:H	2.22	0.41
1:B:382:ILE:HA	1:B:383:PRO:HD3	1.72	0.41
1:A:436:CYS:HA	2:A:500:HEM:CHA	2.50	0.41
1:B:429:PHE:HB3	1:B:436:CYS:HB3	2.01	0.41
1:B:85:ARG:NH2	1:B:424:GLU:HB3	2.35	0.41
1:B:134:ASP:O	1:B:137:MET:CB	2.69	0.41
1:A:43:LEU:HA	1:A:43:LEU:HD12	1.76	0.41
1:B:151:GLN:HA	1:B:154:ILE:HG12	2.03	0.41
1:A:110:GLY:C	1:A:120:ARG:HH11	2.24	0.41
3:A:501:06X:CAV	3:A:501:06X:H18	2.51	0.41
3:A:502:06X:CAV	3:A:502:06X:CAK	2.93	0.41
1:B:178:ILE:O	1:B:182:ILE:HG13	2.21	0.41
1:A:437:LEU:CB	2:A:500:HEM:CMD	2.99	0.41
1:A:232:ARG:CZ	1:B:262:ARG:HD3	2.50	0.41
3:B:501:06X:OAS	3:B:501:06X:CAK	2.68	0.41
1:A:98:ARG:NH1	1:A:367:VAL:CG1	2.83	0.41
1:B:35:ARG:HH21	1:B:37:LEU:HD21	1.86	0.41
2:B:500:HEM:CMB	2:B:500:HEM:CBB	2.69	0.41
1:A:489:LEU:HA	1:A:490:PRO:HD3	1.91	0.40
2:A:500:HEM:CMB	2:A:500:HEM:HBB2	2.51	0.40
1:B:300:THR:O	3:B:501:06X:H16	2.21	0.40
1:A:384:LYS:HG2	1:A:385:ASP:OD1	2.21	0.40
1:B:202:PHE:O	1:B:203:TYR:C	2.58	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ASP:HA	1:A:399:PRO:HD3	1.97	0.40
1:A:448:LEU:HD23	1:A:448:LEU:HA	1.85	0.40
1:B:136:GLY:H	1:B:139:LYS:HZ3	1.69	0.40
1:B:336:ARG:HH22	1:B:342:ASP:CG	2.24	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	464/476 (98%)	430 (93%)	32 (7%)	2 (0%)	34	66
1	B	458/476 (96%)	433 (94%)	25 (6%)	0	100	100
All	All	922/952 (97%)	863 (94%)	57 (6%)	2 (0%)	47	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	GLY
1	A	411	ASP

### 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	390/418 (93%)	380 (97%)	10 (3%)	46 79
1	B	388/418 (93%)	379 (98%)	9 (2%)	50 82
All	All	778/836 (93%)	759 (98%)	19 (2%)	49 81

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	LYS
1	A	140	ARG
1	A	215	GLN
1	A	268	TYR
1	A	301	GLU
1	A	302	THR
1	A	309	TYR
1	A	371	VAL
1	A	403	GLU
1	A	435	ILE
1	B	53	LYS
1	B	90	ASP
1	B	139	LYS
1	B	140	ARG
1	B	302	THR
1	B	309	TYR
1	B	371	VAL
1	B	387	GLU
1	B	403	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	237	ASN
1	B	335	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 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	$\# Z  > 2$
3	06X	B	501	2	29,29,29	3.75	11 (37%)	37,39,39	2.71	10 (27%)
3	06X	B	502	-	29,29,29	3.74	11 (37%)	37,39,39	2.74	11 (29%)
2	HEM	B	500	1,3	27,50,50	2.96	10 (37%)	17,82,82	2.38	5 (29%)
2	HEM	A	500	1,3	27,50,50	2.86	10 (37%)	17,82,82	2.15	5 (29%)
3	06X	A	502	-	29,29,29	3.74	11 (37%)	37,39,39	2.72	10 (27%)
3	06X	A	501	2	29,29,29	3.74	11 (37%)	37,39,39	2.72	10 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	06X	B	501	2	-	4/22/42/42	0/2/2/2
3	06X	B	502	-	-	7/22/42/42	0/2/2/2
2	HEM	B	500	1,3	-	2/6/54/54	-
2	HEM	A	500	1,3	-	0/6/54/54	-
3	06X	A	502	-	-	5/22/42/42	0/2/2/2
3	06X	A	501	2	-	3/22/42/42	0/2/2/2

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	06X	CBA-CBB	-9.31	1.39	1.53
3	B	501	06X	CBA-CBB	-9.30	1.39	1.53
3	A	501	06X	CBA-CBB	-9.29	1.39	1.53
3	A	502	06X	CBA-CBB	-9.28	1.39	1.53
3	A	501	06X	CBB-CAX	-9.22	1.39	1.52
3	B	501	06X	CBB-CAX	-9.19	1.39	1.52
3	B	502	06X	CBB-CAX	-9.18	1.39	1.52
3	A	502	06X	CBB-CAX	-9.14	1.39	1.52
2	A	500	HEM	C3C-C2C	-9.05	1.27	1.40
2	B	500	HEM	C3C-C2C	-8.98	1.27	1.40
2	B	500	HEM	C3B-C2B	-8.90	1.28	1.40
3	B	502	06X	CBB-CAY	-8.86	1.39	1.52
3	B	501	06X	CBB-CAY	-8.84	1.39	1.52
3	A	502	06X	CBB-CAY	-8.80	1.39	1.52
3	A	501	06X	CBB-CAY	-8.72	1.40	1.52
2	A	500	HEM	C3B-C2B	-8.11	1.29	1.40
3	A	501	06X	CAO-CAW	-6.37	1.39	1.50
3	A	501	06X	CAC-CAT	-6.35	1.39	1.49
3	B	502	06X	CAC-CAT	-6.33	1.39	1.49
3	B	501	06X	CAO-CAW	-6.32	1.39	1.50
3	A	502	06X	CAC-CAT	-6.32	1.39	1.49
3	A	502	06X	CAO-CAW	-6.31	1.39	1.50
3	B	501	06X	CAC-CAT	-6.30	1.39	1.49
3	B	502	06X	CAO-CAW	-6.30	1.39	1.50
3	A	501	06X	CAU-CAX	-4.14	1.39	1.47
3	A	502	06X	CAU-CAX	-4.14	1.39	1.47
3	B	502	06X	CAU-CAX	-4.11	1.39	1.47
3	B	501	06X	CAU-CAX	-4.11	1.39	1.47
3	A	502	06X	CAV-CAY	-3.98	1.39	1.47
3	B	502	06X	CAV-CAY	-3.97	1.39	1.47
3	B	501	06X	CAV-CAY	-3.96	1.39	1.47
3	A	501	06X	CAV-CAY	-3.96	1.39	1.47
3	B	501	06X	CAT-NAP	-3.73	1.33	1.38
3	A	501	06X	CAT-NAP	-3.72	1.33	1.38
3	B	502	06X	CAT-NAP	-3.69	1.33	1.38
3	A	502	06X	CAT-NAP	-3.68	1.33	1.38
2	A	500	HEM	C3D-C2D	3.66	1.48	1.37
2	B	500	HEM	C3D-C2D	3.64	1.48	1.37
2	B	500	HEM	C1D-CHD	-3.46	1.31	1.41
2	B	500	HEM	C4A-CHB	-3.27	1.31	1.41
2	A	500	HEM	C4B-CHC	-3.19	1.32	1.41
2	B	500	HEM	C4B-CHC	-3.14	1.32	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C1D-CHD	-3.13	1.32	1.41
3	A	501	06X	CAT-CAX	3.10	1.39	1.35
3	B	501	06X	CAT-CAX	3.06	1.39	1.35
3	A	502	06X	CAT-CAX	3.05	1.39	1.35
3	B	502	06X	CAT-CAX	3.02	1.39	1.35
2	B	500	HEM	C1A-CHA	-2.87	1.33	1.41
2	A	500	HEM	C3B-CAB	2.75	1.53	1.47
2	A	500	HEM	C4A-CHB	-2.66	1.33	1.41
2	A	500	HEM	C2A-C3A	-2.56	1.30	1.37
2	A	500	HEM	C1A-CHA	-2.53	1.33	1.41
3	B	501	06X	CAW-CAY	2.53	1.39	1.36
2	B	500	HEM	C2A-C3A	-2.52	1.30	1.37
3	B	501	06X	CAW-NAP	-2.51	1.33	1.37
3	A	502	06X	CAW-CAY	2.50	1.39	1.36
3	A	502	06X	CAW-NAP	-2.49	1.33	1.37
3	B	502	06X	CAW-CAY	2.49	1.39	1.36
3	B	502	06X	CAW-NAP	-2.48	1.33	1.37
2	A	500	HEM	C3C-CAC	2.44	1.52	1.47
3	A	501	06X	CAW-CAY	2.42	1.39	1.36
3	A	501	06X	CAW-NAP	-2.41	1.33	1.37
2	B	500	HEM	C3B-CAB	2.36	1.52	1.47
2	B	500	HEM	C3C-CAC	2.27	1.52	1.47

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	06X	CAT-NAP-CAW	-12.44	112.08	122.43
3	A	502	06X	CAT-NAP-CAW	-12.41	112.10	122.43
3	B	502	06X	CAT-NAP-CAW	-12.40	112.11	122.43
3	B	501	06X	CAT-NAP-CAW	-12.39	112.12	122.43
2	A	500	HEM	CAD-CBD-CGD	-6.63	101.54	112.67
2	B	500	HEM	C1D-C2D-C3D	-5.54	103.14	107.00
2	B	500	HEM	CAD-CBD-CGD	-5.16	104.02	112.67
3	B	502	06X	CAL-OAS-CAV	-3.98	109.44	116.50
3	B	501	06X	CAL-OAS-CAV	-3.97	109.47	116.50
3	A	501	06X	CAL-OAS-CAV	-3.95	109.49	116.50
3	A	502	06X	CAL-OAS-CAV	-3.94	109.52	116.50
3	A	501	06X	CAC-CAT-CAX	-3.76	123.86	127.62
3	A	502	06X	CAC-CAT-CAX	-3.75	123.87	127.62
2	B	500	HEM	CAA-CBA-CGA	-3.75	106.38	112.67
3	B	501	06X	CAC-CAT-CAX	-3.73	123.89	127.62
3	B	502	06X	CAC-CAT-CAX	-3.72	123.90	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	06X	CAC-CAT-NAP	3.63	117.77	113.45
3	A	502	06X	CAC-CAT-NAP	3.60	117.73	113.45
3	B	502	06X	CAC-CAT-NAP	3.60	117.73	113.45
3	B	501	06X	CAC-CAT-NAP	3.59	117.73	113.45
3	B	502	06X	CAB-OAQ-CAU	-3.38	109.47	115.86
3	A	502	06X	CAB-OAQ-CAU	-3.37	109.49	115.86
3	B	501	06X	CAB-OAQ-CAU	-3.36	109.51	115.86
3	A	501	06X	CAB-OAQ-CAU	-3.36	109.51	115.86
3	A	502	06X	CAK-CBA-CAZ	3.25	120.04	116.81
3	A	501	06X	CAK-CBA-CAZ	3.23	120.02	116.81
2	A	500	HEM	C3B-C4B-NB	3.22	113.38	109.21
3	B	501	06X	CAK-CBA-CAZ	3.21	120.00	116.81
3	B	502	06X	CAK-CBA-CAZ	3.17	119.97	116.81
2	B	500	HEM	C3B-C4B-NB	3.07	113.18	109.21
3	A	502	06X	CAZ-CBA-CBB	-3.00	119.98	123.98
3	B	502	06X	CAZ-CBA-CBB	-3.00	119.98	123.98
3	A	501	06X	CAZ-CBA-CBB	-2.99	120.00	123.98
3	B	501	06X	CAZ-CBA-CBB	-2.97	120.02	123.98
2	A	500	HEM	CAA-CBA-CGA	-2.47	108.53	112.67
2	A	500	HEM	C1D-C2D-C3D	-2.46	105.28	107.00
3	B	502	06X	OAS-CAL-CAA	2.39	117.20	108.42
3	B	501	06X	OAF-CAV-CAY	-2.31	120.42	125.20
3	A	502	06X	OAF-CAV-CAY	-2.31	120.43	125.20
3	A	501	06X	OAF-CAV-CAY	-2.30	120.43	125.20
3	B	502	06X	OAF-CAV-CAY	-2.27	120.49	125.20
2	B	500	HEM	CMD-C2D-C3D	2.26	129.20	124.94
3	A	502	06X	CAJ-CAZ-CBA	-2.22	119.98	121.99
3	A	501	06X	CAJ-CAZ-CBA	-2.20	119.99	121.99
2	A	500	HEM	CBD-CAD-C3D	-2.17	108.48	112.48
3	B	501	06X	CAJ-CAZ-CBA	-2.17	120.02	121.99
3	B	502	06X	CAJ-CAZ-CBA	-2.17	120.02	121.99
3	A	501	06X	OAS-CAV-CAY	2.12	116.09	112.31
3	A	502	06X	OAS-CAV-CAY	2.10	116.06	112.31
3	B	502	06X	OAS-CAV-CAY	2.10	116.05	112.31
3	B	501	06X	OAS-CAV-CAY	2.10	116.05	112.31

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	06X	NAD-CAM-CAN-OAR
3	A	501	06X	NAD-CAM-CAN-OAR

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Mol	Chain	Res	Type	Atoms
3	B	501	06X	CAX-CAU-OAQ-CAB
3	B	502	06X	CAY-CAV-OAS-CAL
3	B	502	06X	OAF-CAV-OAS-CAL
3	A	502	06X	CAY-CAV-OAS-CAL
3	B	501	06X	OAE-CAU-OAQ-CAB
3	A	502	06X	OAF-CAV-OAS-CAL
3	B	502	06X	CAX-CAU-OAQ-CAB
3	B	502	06X	OAE-CAU-OAQ-CAB
3	A	502	06X	CAX-CAU-OAQ-CAB
3	A	502	06X	OAE-CAU-OAQ-CAB
3	B	502	06X	CAW-CAO-OAR-CAN
2	B	500	HEM	C2D-C3D-CAD-CBD
2	B	500	HEM	C4D-C3D-CAD-CBD
3	A	501	06X	CAM-CAN-OAR-CAO
3	B	501	06X	CAM-CAN-OAR-CAO
3	B	501	06X	OAR-CAO-CAW-NAP
3	A	501	06X	OAR-CAO-CAW-NAP
3	A	502	06X	CAA-CAL-OAS-CAV
3	B	502	06X	OAR-CAO-CAW-CAY

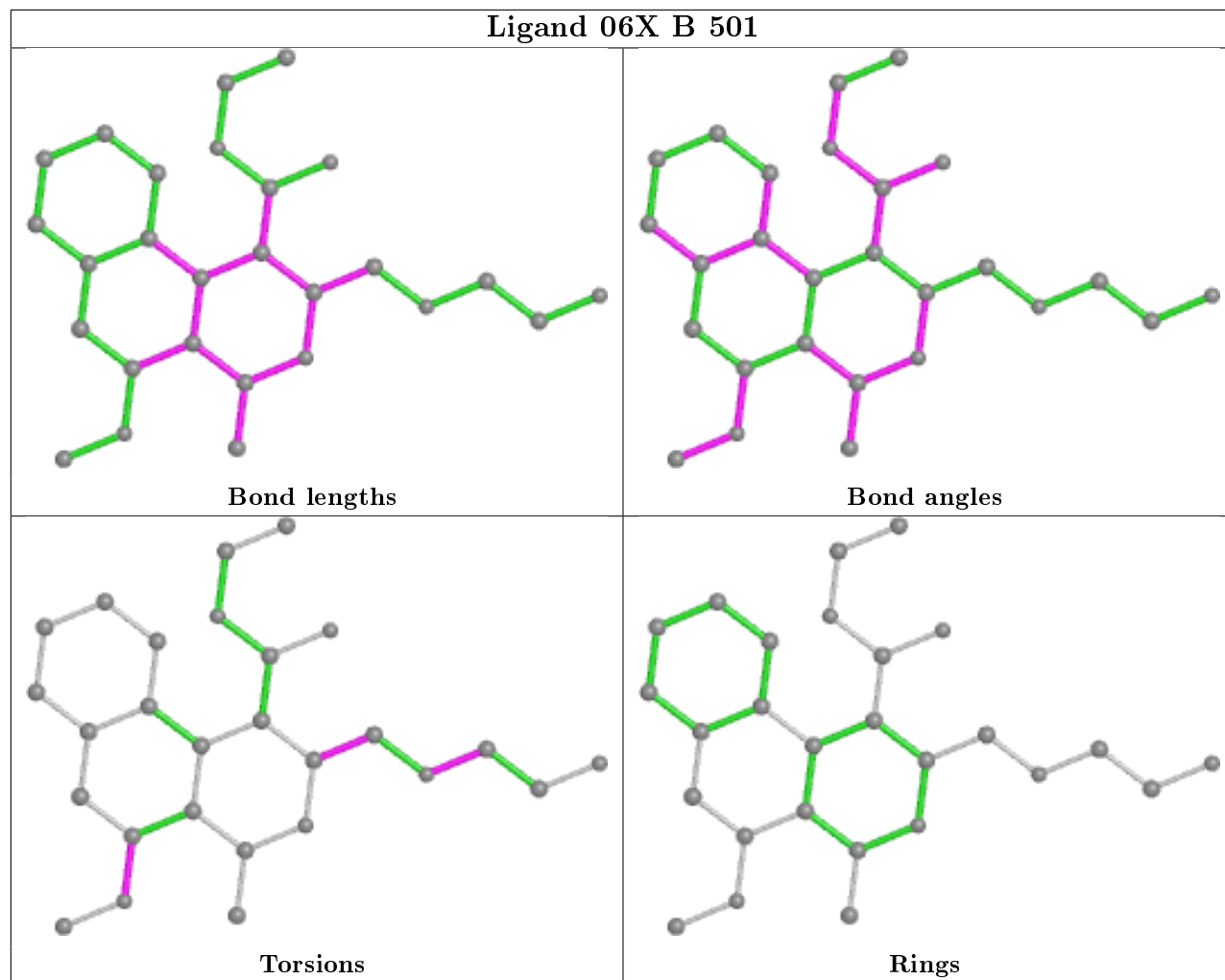
There are no ring outliers.

6 monomers are involved in 116 short contacts:

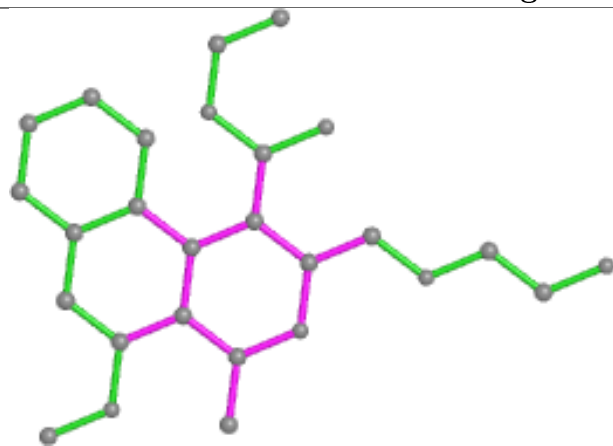
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	06X	18	0
3	B	502	06X	19	0
2	B	500	HEM	20	0
2	A	500	HEM	22	0
3	A	502	06X	23	0
3	A	501	06X	14	0

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

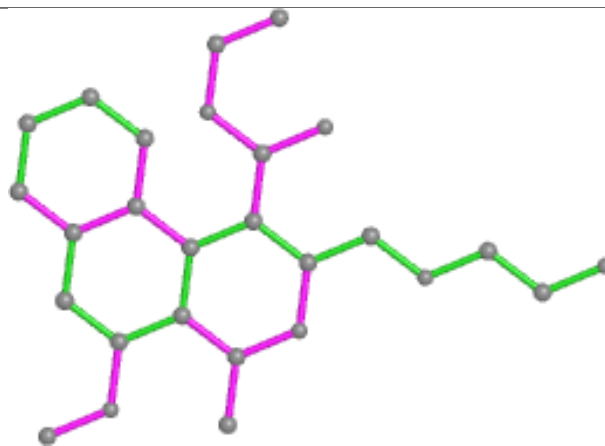
equivalents in the CSD to analyse the geometry.



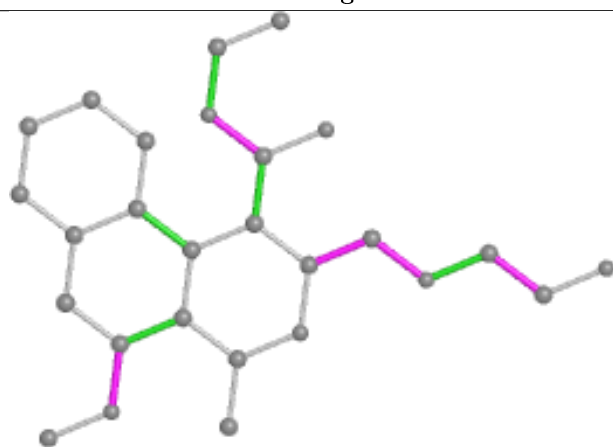
## Ligand 06X B 502



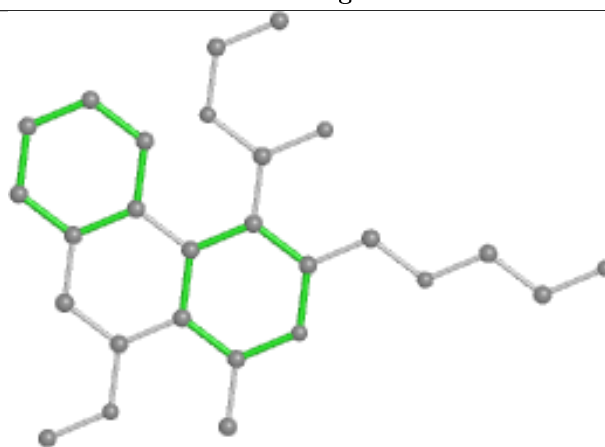
Bond lengths



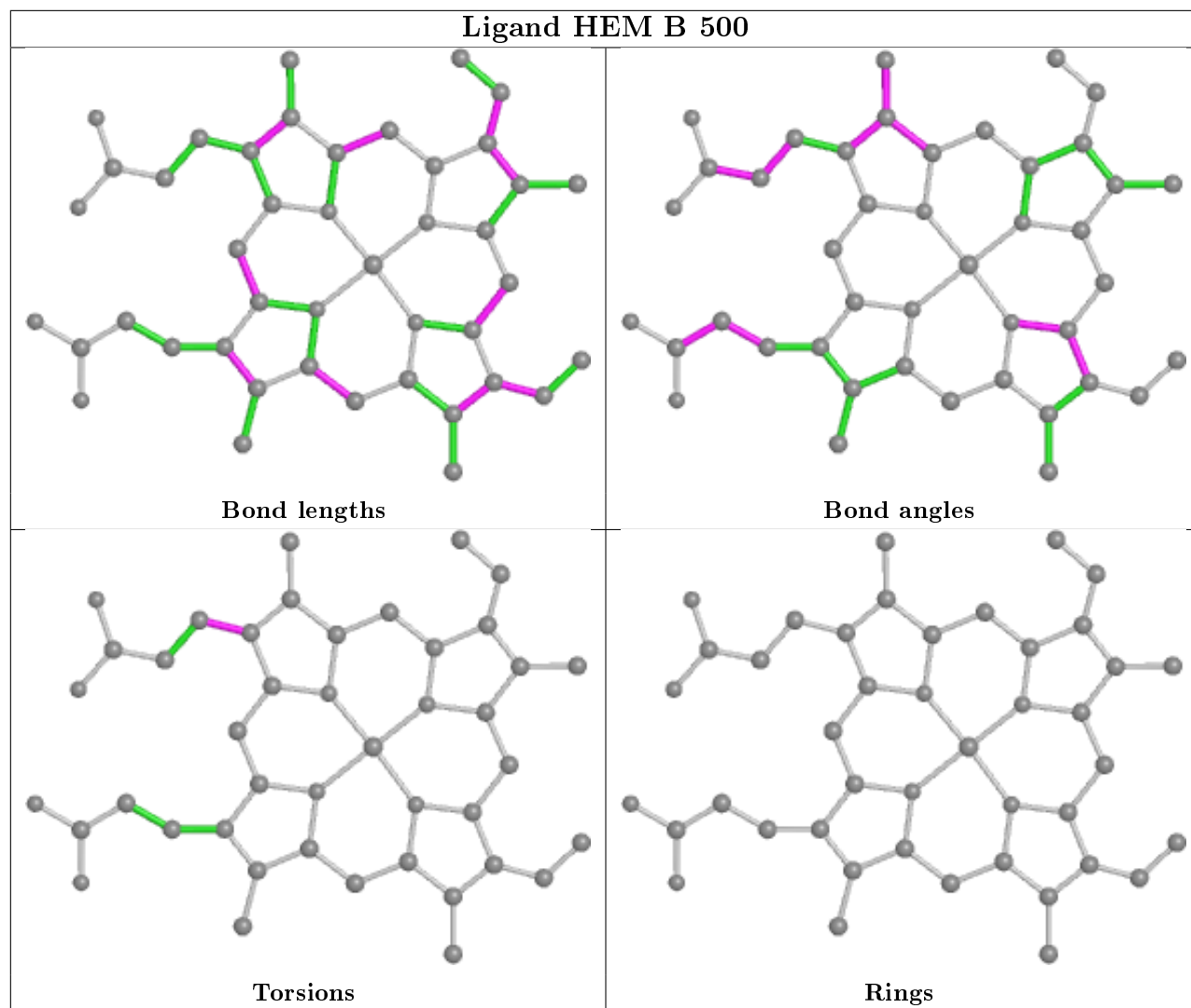
Bond angles

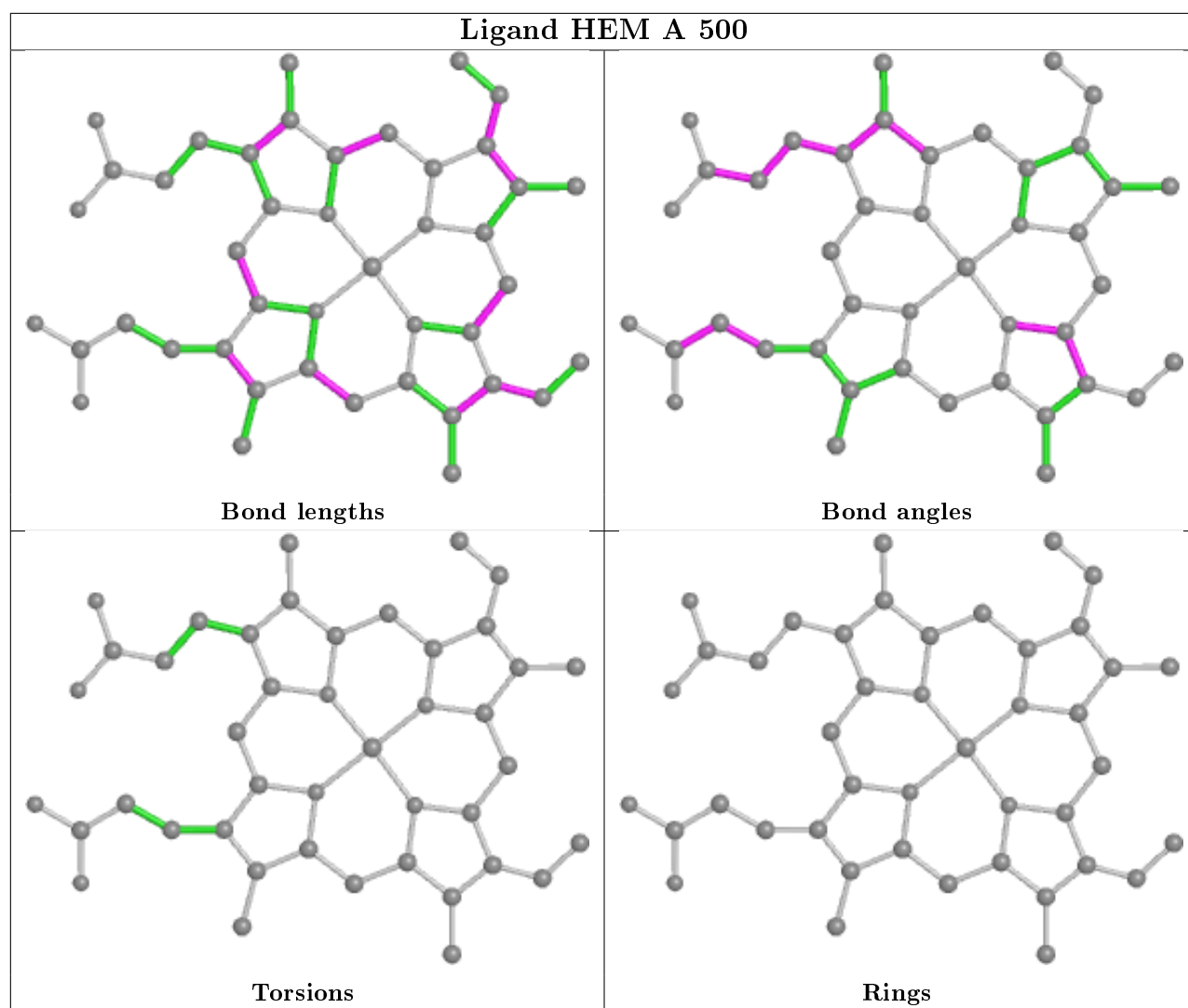


Torsions

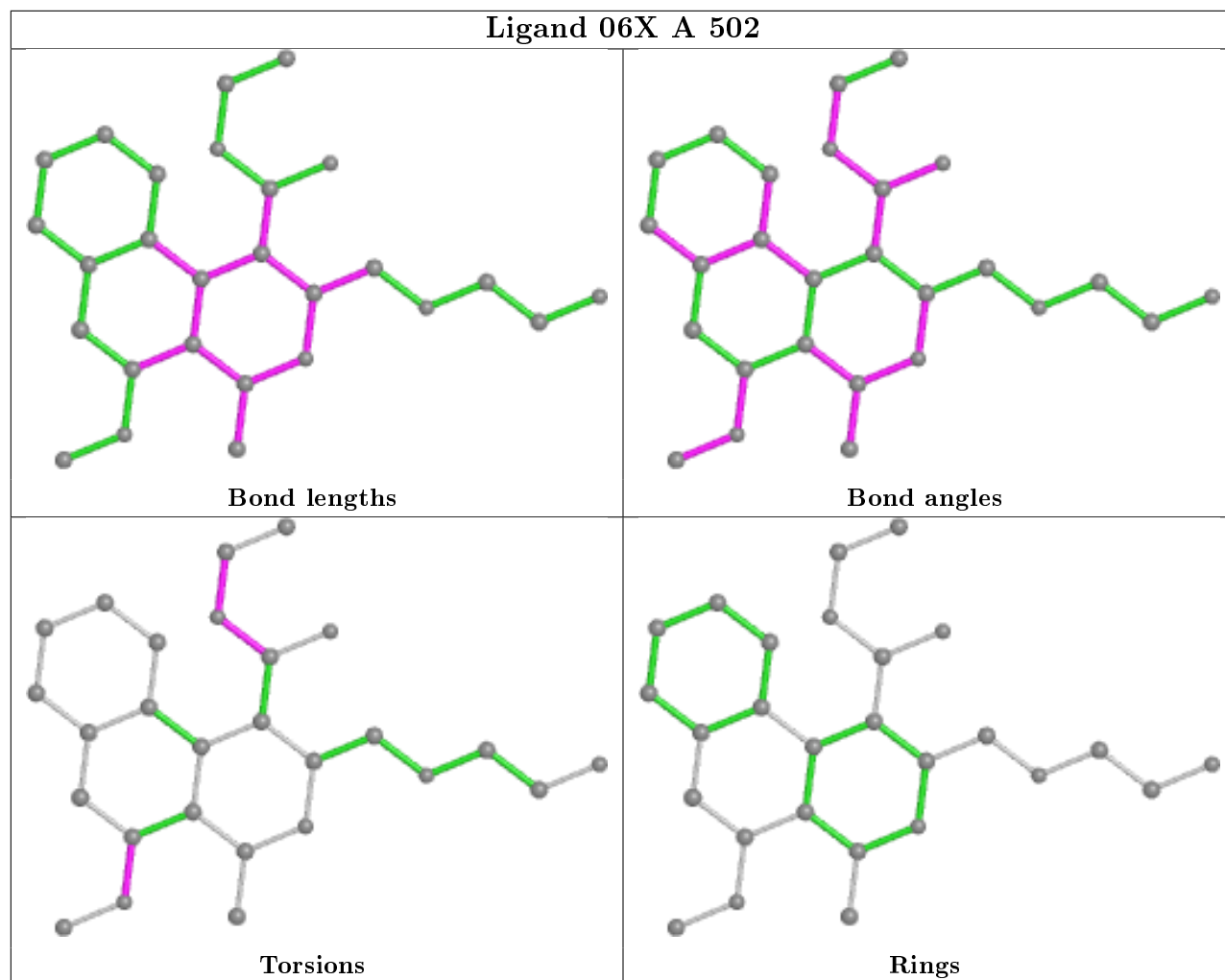


Rings

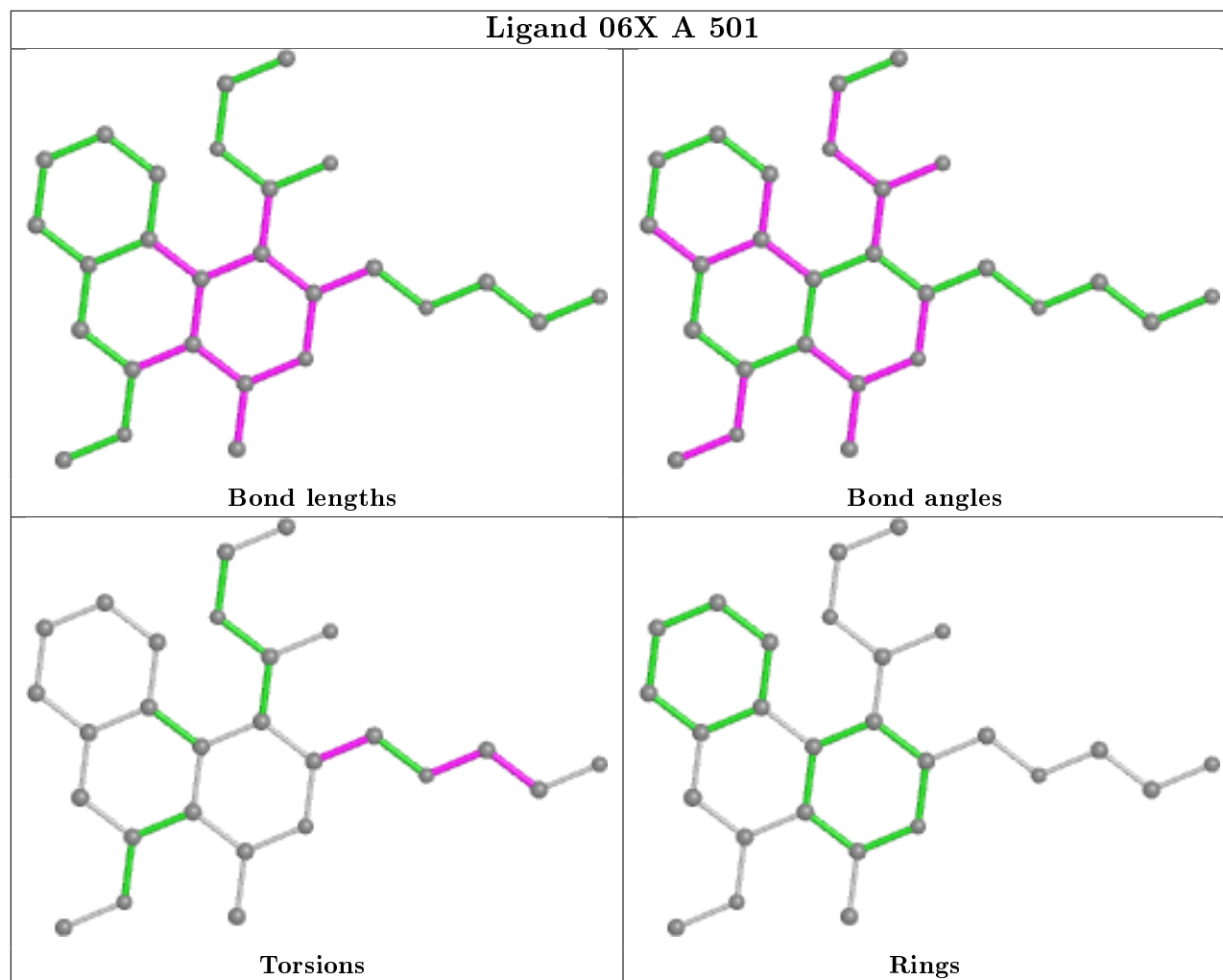




## Ligand 06X A 502







## 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 [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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	465/476 (97%)	0.04	4 (0%) 84 80	27, 50, 69, 79	0
1	B	462/476 (97%)	-0.04	6 (1%) 77 72	33, 50, 68, 80	0
All	All	927/952 (97%)	0.00	10 (1%) 80 75	27, 50, 69, 80	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	56	LEU	2.8
1	B	193	GLN	2.5
1	A	492	HIS	2.3
1	B	277	SER	2.3
1	B	283	PHE	2.2
1	A	222	GLY	2.2
1	A	228	PRO	2.2
1	B	321	ALA	2.1
1	A	323	ARG	2.1
1	B	230	ALA	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 carbohydrates in this entry.

## 6.4 Ligands

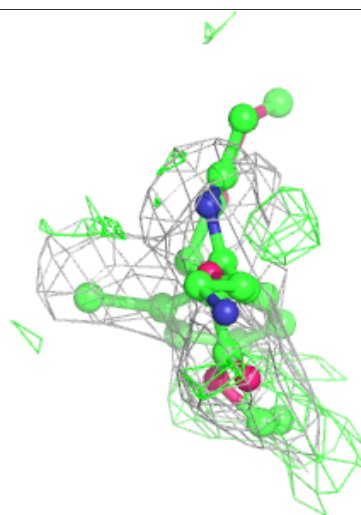
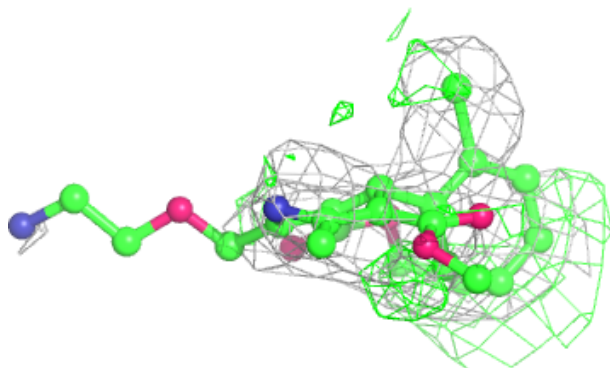
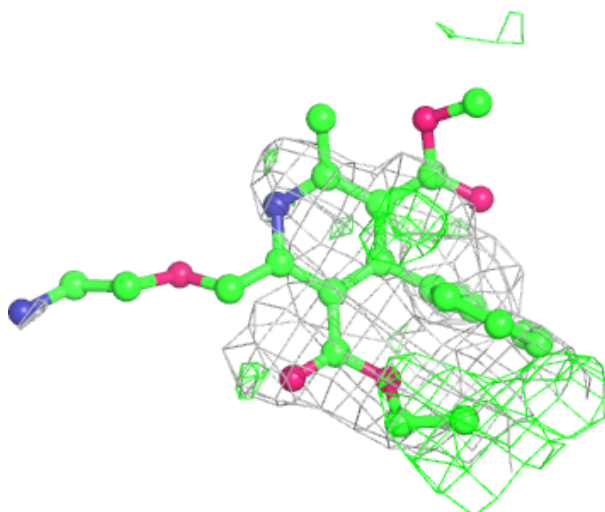
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	06X	A	502	28/28	0.69	0.46	54,66,69,73	28
3	06X	B	502	28/28	0.82	0.28	55,66,73,73	0
3	06X	B	501	28/28	0.90	0.22	38,48,52,57	0
3	06X	A	501	28/28	0.90	0.28	32,48,53,56	0
2	HEM	A	500	43/43	0.96	0.16	31,39,44,45	0
2	HEM	B	500	43/43	0.97	0.18	35,38,40,42	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.

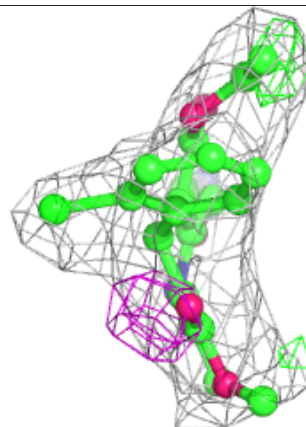
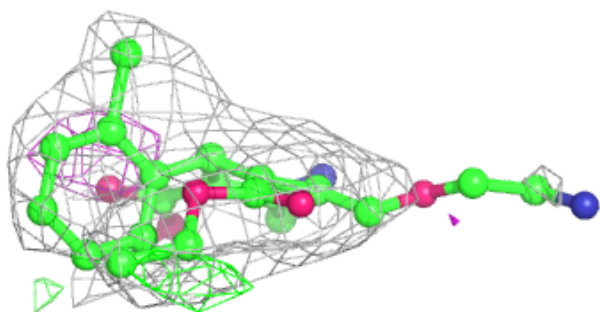
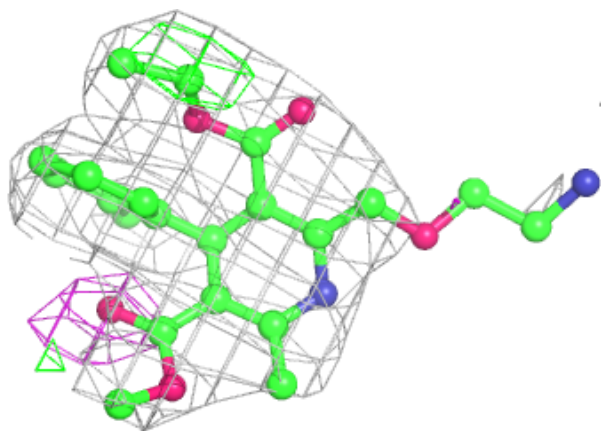
**Electron density around 06X A 502:**

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



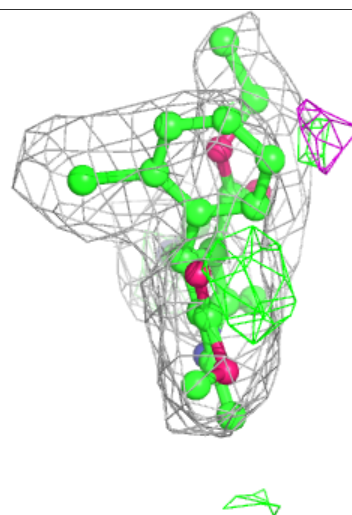
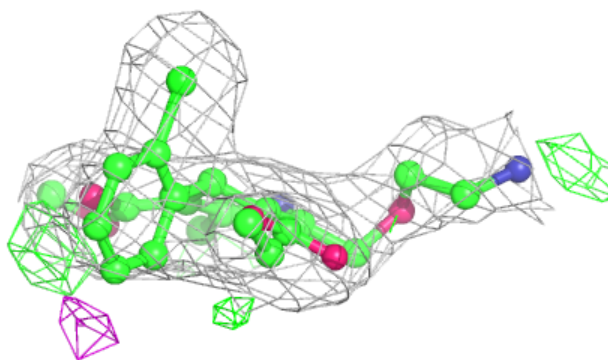
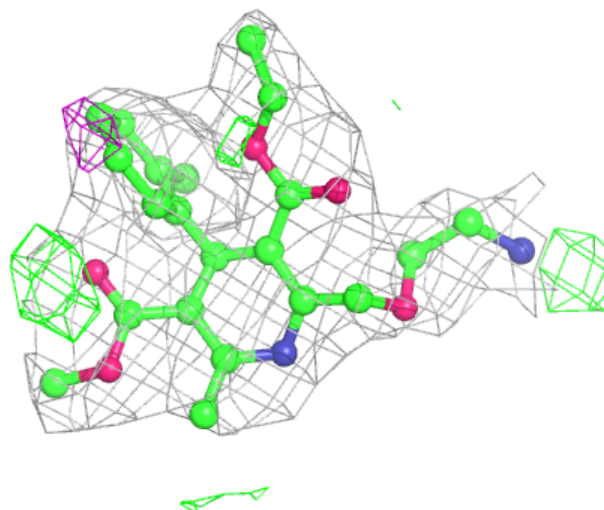
**Electron density around 06X B 502:**

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



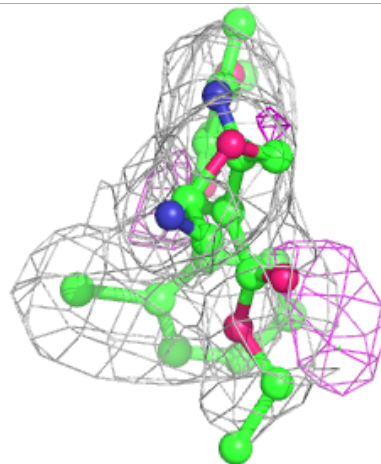
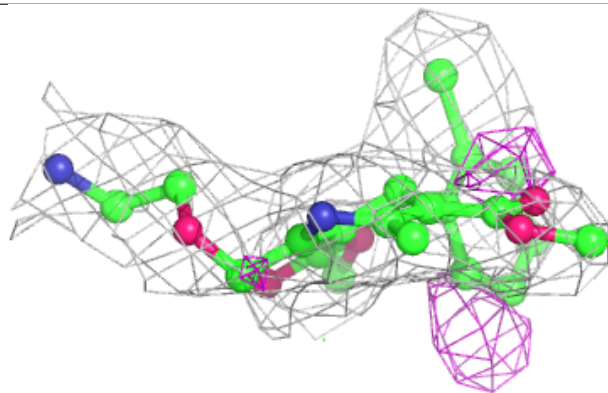
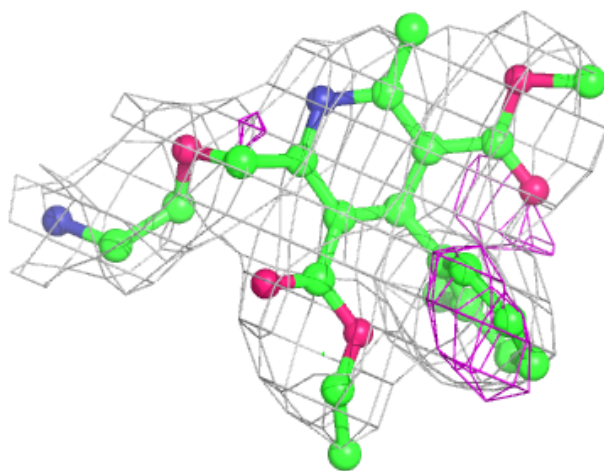
**Electron density around 06X B 501:**

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



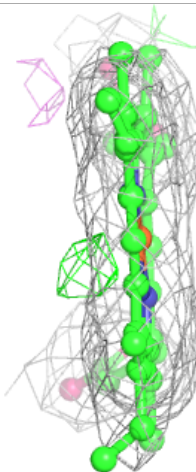
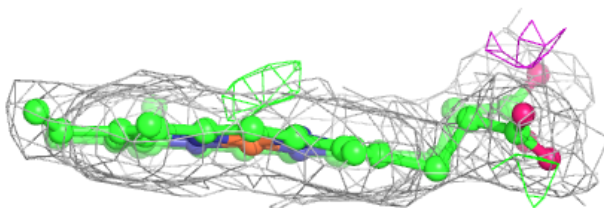
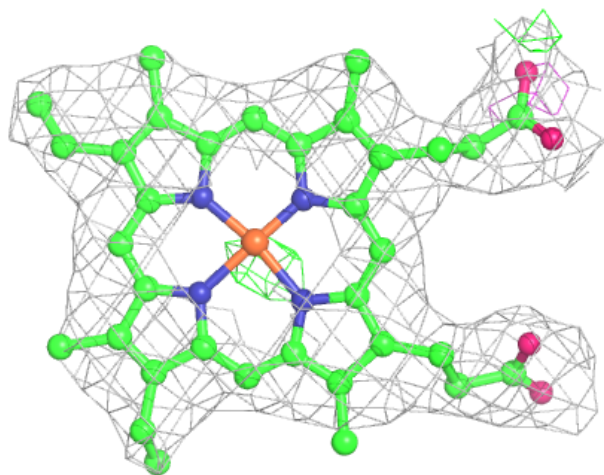
**Electron density around 06X A 501:**

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

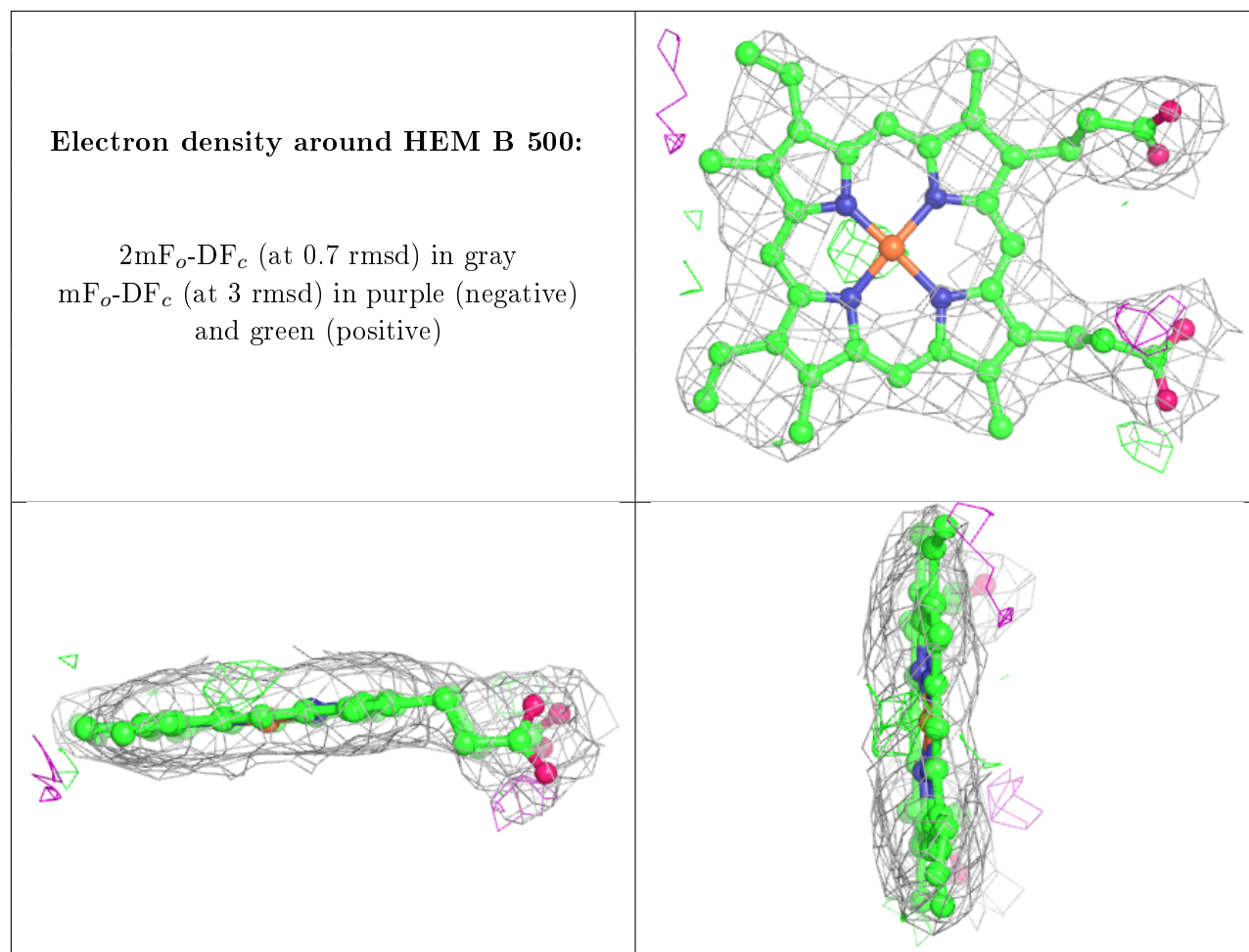


**Electron density around HEM A 500:**

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







## 6.5 Other polymers ⓘ

There are no such residues in this entry.