



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:56 pm BST

PDB ID : 2FDY  
Title : Microsomal P450 2A6 with the inhibitor Adrithiol bound  
Authors : Yano, J.K.; Stout, C.D.; Johnson, E.F.  
Deposited on : 2005-12-14  
Resolution : 1.95 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

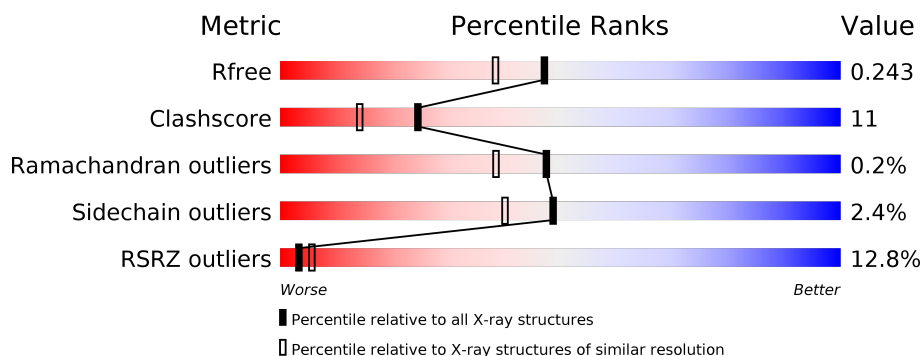
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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>9%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
1	B	476	<div> <div>15%</div> <div>70%</div> <div>25%</div> <div>..</div> </div>
1	C	476	<div> <div>10%</div> <div>76%</div> <div>21%</div> <div>..</div> </div>
1	D	476	<div> <div>16%</div> <div>75%</div> <div>22%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	D4G	A	501	-	X	-	-
4	D4G	B	501	-	X	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16035 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
1	A	465	Total	C	N	O	S	0	0	0
			3760	2414	650	678	18			
1	B	464	Total	C	N	O	S	0	0	0
			3757	2412	650	677	18			
1	C	464	Total	C	N	O	S	0	0	0
			3751	2408	648	677	18			
1	D	464	Total	C	N	O	S	0	0	0
			3751	2408	648	677	18			

There are 40 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	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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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	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 SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



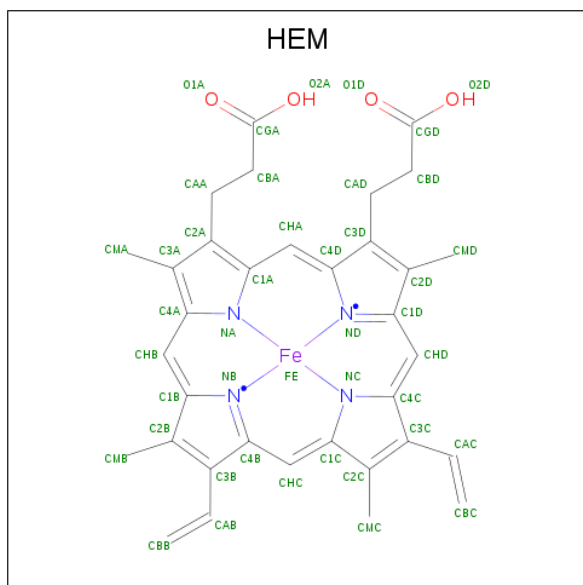
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

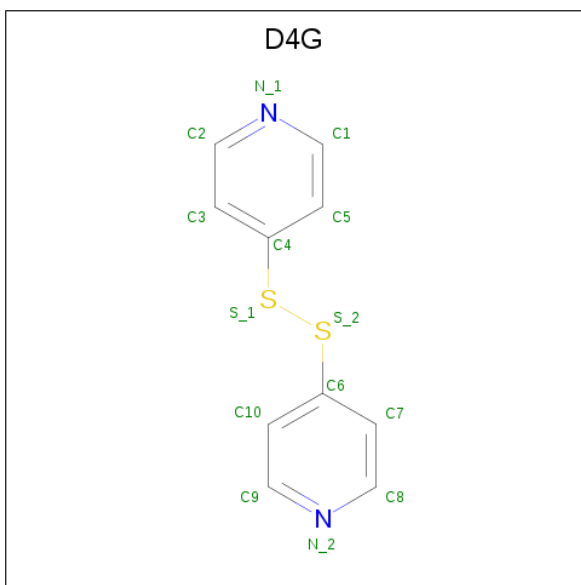
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	S	0	0
			14	10	2	2		
4	B	1	Total	C	N	S	0	0
			14	10	2	2		
4	C	1	Total	C	N	S	0	0
			14	10	2	2		
4	D	1	Total	C	N	S	0	0
			14	10	2	2		

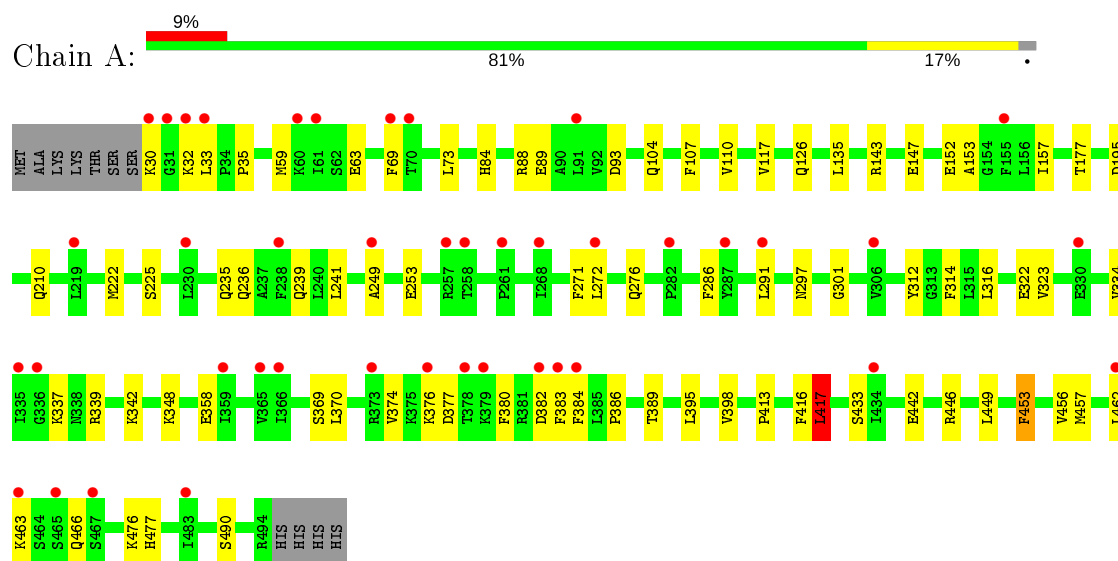
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	232	Total	O	0	0
			232	232		
5	B	139	Total	O	0	0
			139	139		
5	C	224	Total	O	0	0
			224	224		
5	D	178	Total	O	0	0
			178	178		

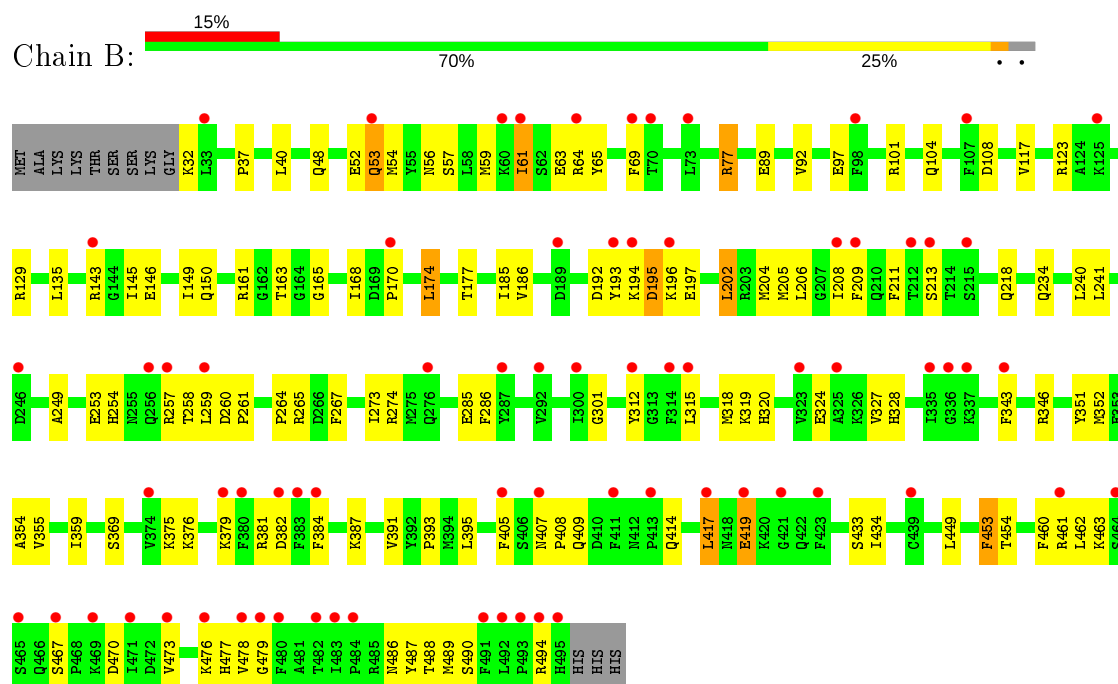
### 3 Residue-property plots [i](#)

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 2A6

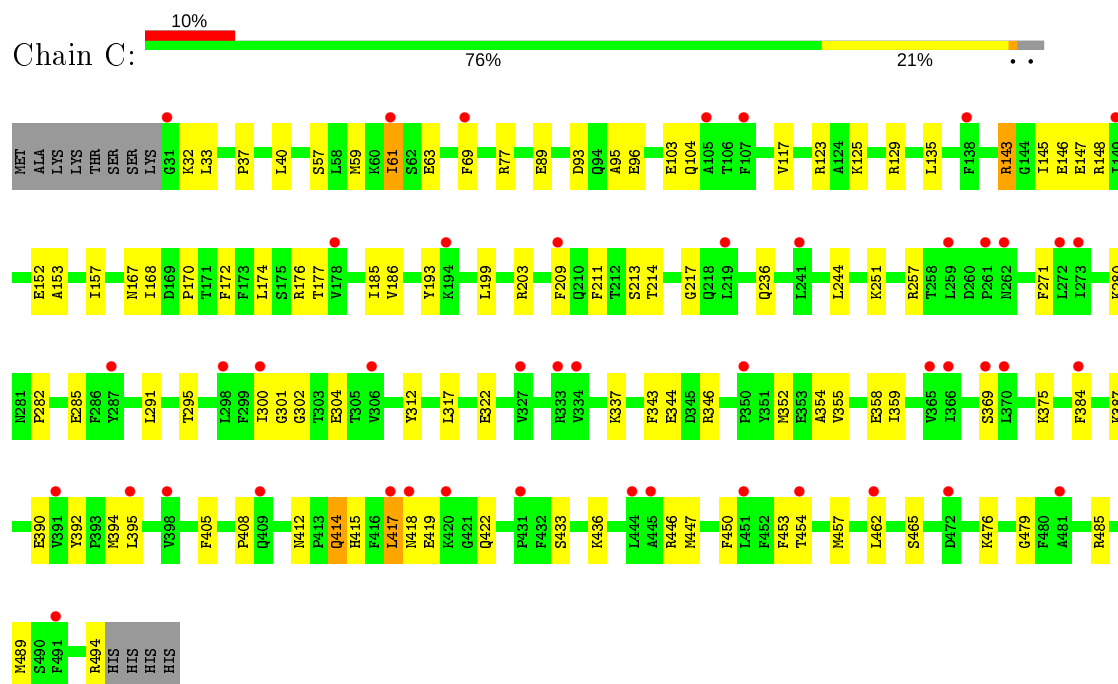


#### • Molecule 1: Cytochrome P450 2A6

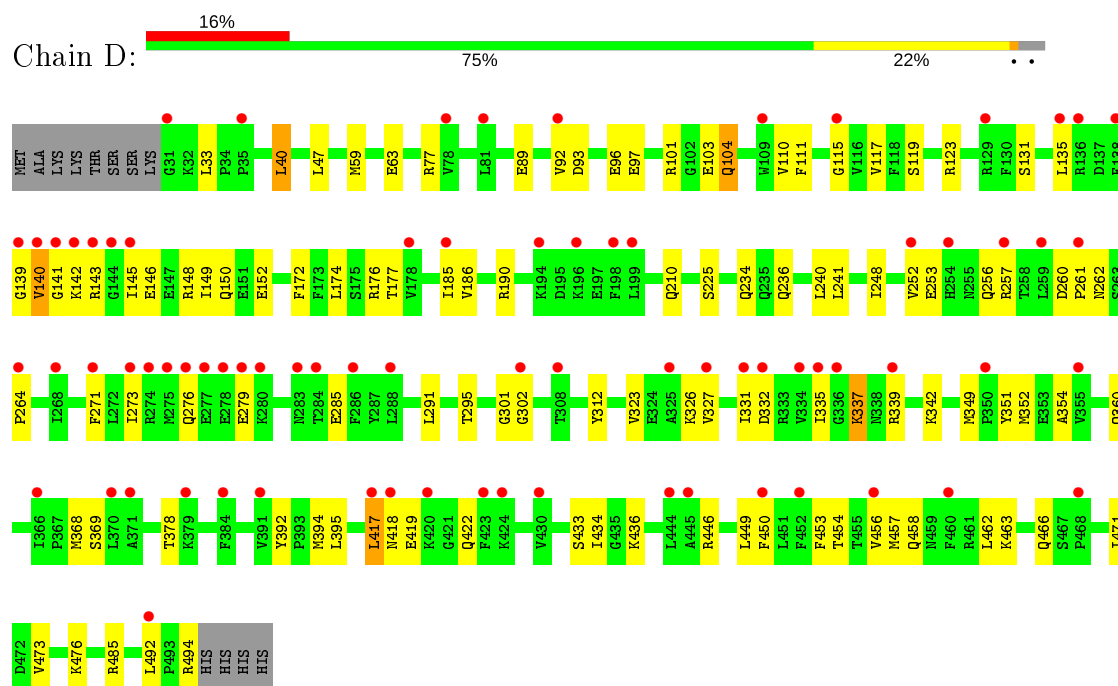




• Molecule 1: Cytochrome P450 2A6



• Molecule 1: Cytochrome P450 2A6



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.20 Å 156.62 Å 104.00 Å 90.00° 91.79° 90.00°	Depositor
Resolution (Å)	42.41 – 1.95 42.40 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.7 (42.41-1.95) 97.5 (42.40-1.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.49 (at 1.89 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.212 , 0.250 0.207 , 0.243	Depositor DCC
$R_{free}$ test set	8609 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.3	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 54.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16035	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, D4G, SO4

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	0.37	0/3851	0.59	2/5186 (0.0%)
1	B	0.34	0/3849	0.56	1/5185 (0.0%)
1	C	0.38	0/3842	0.59	1/5175 (0.0%)
1	D	0.36	0/3842	0.59	1/5175 (0.0%)
All	All	0.36	0/15384	0.58	5/20721 (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	104	GLN	N-CA-C	-5.67	95.70	111.00
1	D	104	GLN	N-CA-C	-5.57	95.95	111.00
1	B	104	GLN	N-CA-C	-5.36	96.53	111.00
1	A	417	LEU	CA-CB-CG	5.30	127.50	115.30
1	C	104	GLN	N-CA-C	-5.27	96.78	111.00

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	3760	0	3747	55	0
1	B	3757	0	3738	114	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3751	0	3734	74	0
1	D	3751	0	3734	89	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
3	A	43	0	30	3	0
3	B	43	0	30	2	0
3	C	43	0	30	4	0
3	D	43	0	30	4	0
4	A	14	0	8	4	0
4	B	14	0	8	1	0
4	C	14	0	8	1	0
4	D	14	0	8	3	0
5	A	232	0	0	2	0
5	B	139	0	0	7	0
5	C	224	0	0	4	0
5	D	178	0	0	3	0
All	All	16035	0	15105	331	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 11.

All (331) 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:32:LYS:HB3	1:C:384:PHE:HB3	1.45	0.97
1:D:463:LYS:HD3	1:D:492:LEU:HD11	1.52	0.91
1:B:352:MET:HE3	1:B:454:THR:HG22	1.54	0.87
1:B:77:ARG:HG2	1:B:77:ARG:HH11	1.40	0.86
1:B:61:ILE:HD11	1:B:69:PHE:CD1	2.12	0.84
1:B:208:ILE:HD11	1:B:240:LEU:HB2	1.60	0.83
1:C:412:ASN:OD1	1:C:414:GLN:HB2	1.80	0.82
1:B:375:LYS:HE2	5:B:2610:HOH:O	1.82	0.79
1:B:407:ASN:HB3	1:B:409:GLN:HE22	1.47	0.78
1:B:318:MET:HE1	1:B:489:MET:HB2	1.64	0.77
1:B:407:ASN:HB3	1:B:409:GLN:NE2	2.00	0.76
1:B:414:GLN:NE2	1:B:417:LEU:HD23	2.00	0.76
1:B:258:THR:HG23	1:B:265:ARG:HH22	1.51	0.75
1:C:392:TYR:HB3	1:C:394:MET:CE	2.17	0.75
1:A:235:GLN:O	1:A:239:GLN:HG2	1.87	0.74
1:D:418:ASN:HD22	1:D:422:GLN:HB2	1.53	0.73
1:D:392:TYR:HB3	1:D:394:MET:HE3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:PHE:O	1:C:214:THR:HG22	1.87	0.73
1:C:37:PRO:HD3	1:C:61:ILE:HD13	1.73	0.71
1:C:125:LYS:HZ2	1:C:129:ARG:NH2	1.87	0.71
1:C:61:ILE:HD11	1:C:69:PHE:CD1	2.26	0.71
1:D:392:TYR:HB3	1:D:394:MET:CE	2.21	0.70
1:D:326:LYS:HD2	1:D:351:TYR:CE1	2.27	0.69
1:C:199:LEU:HG	1:C:203:ARG:HH11	1.56	0.69
1:D:101:ARG:HD3	1:D:117:VAL:O	1.93	0.69
1:D:418:ASN:ND2	1:D:422:GLN:HB2	2.08	0.69
1:B:463:LYS:HB3	1:B:490:SER:OG	1.94	0.67
1:C:59:MET:O	1:C:63:GLU:HG3	1.93	0.67
1:B:57:SER:O	1:B:61:ILE:HG23	1.95	0.67
1:C:199:LEU:HG	1:C:203:ARG:NH1	2.10	0.67
1:A:89:GLU:O	1:A:93:ASP:HB2	1.95	0.67
1:B:108:ASP:HB3	5:B:2613:HOH:O	1.94	0.66
1:C:392:TYR:HB3	1:C:394:MET:HE3	1.77	0.66
1:C:125:LYS:NZ	1:C:129:ARG:HH22	1.93	0.66
1:B:494:ARG:HH11	1:B:494:ARG:HG3	1.61	0.66
1:B:193:TYR:CD1	1:B:194:LYS:HG2	2.32	0.65
1:C:352:MET:HE3	1:C:454:THR:HG22	1.78	0.64
1:D:142:LYS:O	1:D:145:ILE:HG22	1.98	0.64
1:D:446:ARG:HG2	5:D:673:HOH:O	1.98	0.63
1:A:457:MET:HE1	1:A:462:LEU:HD21	1.79	0.62
1:D:457:MET:HE1	1:D:462:LEU:HD21	1.82	0.62
1:D:123:ARG:HA	1:D:285:GLU:HG3	1.82	0.62
1:C:123:ARG:HA	1:C:285:GLU:HG3	1.80	0.62
1:C:392:TYR:HB3	1:C:394:MET:HE1	1.81	0.62
1:B:414:GLN:HE22	1:B:417:LEU:HD23	1.64	0.61
1:B:433:SER:HB3	3:B:500:HEM:HBA1	1.81	0.61
1:C:433:SER:HB3	3:C:500:HEM:HBA1	1.82	0.61
1:C:214:THR:HG21	5:C:629:HOH:O	2.00	0.61
1:A:152:GLU:HG3	1:A:177:THR:HG23	1.82	0.61
1:B:476:LYS:HE3	1:B:477:HIS:CD2	2.36	0.61
1:D:419:GLU:CD	1:D:419:GLU:H	2.03	0.61
1:C:117:VAL:HG22	3:C:500:HEM:HAD1	1.82	0.60
1:B:143:ARG:HD2	1:B:146:GLU:OE2	2.01	0.60
1:D:148:ARG:HH21	1:D:190:ARG:HB3	1.66	0.60
1:C:125:LYS:HZ2	1:C:129:ARG:HH22	1.47	0.60
1:B:254:HIS:O	1:B:258:THR:HG22	2.02	0.60
1:D:276:GLN:O	1:D:279:GLU:HB2	2.03	0.59
1:B:318:MET:CE	1:B:489:MET:HB2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:THR:CG2	1:B:265:ARG:HH12	2.16	0.58
1:C:450:PHE:O	1:C:454:THR:HG23	2.04	0.58
1:D:135:LEU:HG	1:D:140:VAL:HG21	1.84	0.58
1:D:101:ARG:CD	1:D:117:VAL:O	2.52	0.58
1:A:210:GLN:HE22	1:A:476:LYS:NZ	2.02	0.58
1:D:139:GLY:HA2	1:D:142:LYS:HE2	1.86	0.58
1:A:433:SER:HB3	3:A:500:HEM:HBA1	1.86	0.57
1:B:208:ILE:CD1	1:B:240:LEU:HB2	2.33	0.57
1:B:161:ARG:HG2	1:B:460:PHE:HZ	1.69	0.57
1:B:213:SER:HA	1:B:479:GLY:HA3	1.87	0.57
1:B:258:THR:HG23	1:B:265:ARG:NH2	2.19	0.57
1:D:271:PHE:CG	1:D:291:LEU:HD13	2.38	0.57
1:A:33:LEU:HD21	1:A:386:PRO:HD2	1.86	0.56
1:D:103:GLU:HG2	1:D:104:GLN:N	2.20	0.56
1:D:252:VAL:O	1:D:256:GLN:HG3	2.05	0.56
1:D:456:VAL:HG12	1:D:457:MET:HE3	1.85	0.56
1:C:152:GLU:HG3	1:C:177:THR:HG23	1.87	0.56
1:A:33:LEU:HD23	1:A:384:PHE:O	2.06	0.56
1:A:271:PHE:HB3	1:A:291:LEU:HD13	1.88	0.56
1:D:326:LYS:HD2	1:D:351:TYR:CZ	2.40	0.56
1:C:418:ASN:HB3	1:C:422:GLN:H	1.71	0.55
1:C:355:VAL:O	1:C:359:ILE:HG13	2.05	0.55
1:B:249:ALA:O	1:B:253:GLU:HG3	2.07	0.55
1:C:170:PRO:O	1:C:174:LEU:HD13	2.07	0.55
1:B:407:ASN:CB	1:B:409:GLN:HE22	2.19	0.55
1:C:405:PHE:O	1:C:408:PRO:HD3	2.05	0.55
1:B:77:ARG:NH1	1:B:77:ARG:HG2	2.14	0.54
1:C:337:LYS:HE2	1:C:494:ARG:NH1	2.22	0.54
1:D:323:VAL:O	1:D:327:VAL:HG23	2.06	0.54
1:C:251:LYS:HZ2	1:C:251:LYS:HB3	1.72	0.54
1:B:196:LYS:O	1:B:196:LYS:HG2	2.06	0.54
1:B:258:THR:HG23	1:B:265:ARG:HH12	1.72	0.54
1:D:97:GLU:OE1	1:D:378:THR:HG23	2.07	0.54
1:D:59:MET:O	1:D:63:GLU:HG3	2.08	0.54
1:B:478:VAL:HG11	5:B:2635:HOH:O	2.08	0.54
1:C:186:VAL:CG1	1:C:295:THR:HG23	2.37	0.54
1:D:337:LYS:NZ	1:D:337:LYS:HB3	2.23	0.54
1:D:458:GLN:O	1:D:494:ARG:HD3	2.08	0.54
1:D:186:VAL:CG1	1:D:295:THR:HG23	2.38	0.54
1:A:73:LEU:HB3	1:A:222:MET:HG2	1.90	0.53
1:C:354:ALA:HB2	1:C:417:LEU:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:SER:HB3	1:B:477:HIS:HB3	1.89	0.53
1:A:30:LYS:HG3	1:A:32:LYS:H	1.73	0.53
1:B:77:ARG:CG	1:B:77:ARG:HH11	2.17	0.53
1:C:280:LYS:O	1:C:282:PRO:HD3	2.09	0.53
1:D:148:ARG:NH2	1:D:190:ARG:HB3	2.22	0.53
1:D:301:GLY:HA2	4:D:501:D4G:C5	2.39	0.53
1:A:334:VAL:HG13	1:A:348:LYS:HE2	1.90	0.53
1:B:193:TYR:HD1	1:B:194:LYS:HG2	1.72	0.53
1:D:110:VAL:HG11	1:D:241:LEU:HD22	1.91	0.53
1:B:414:GLN:HA	1:B:417:LEU:HB2	1.91	0.53
1:C:257:ARG:HH11	1:C:257:ARG:HG2	1.74	0.53
1:C:369:SER:HB2	1:C:395:LEU:HG	1.89	0.53
1:B:264:PRO:HG3	1:B:273:ILE:CD1	2.39	0.53
1:C:214:THR:CG2	1:C:217:GLY:H	2.22	0.53
1:C:103:GLU:HG2	1:C:390:GLU:OE2	2.09	0.53
1:B:163:THR:HG21	1:B:168:ILE:HD13	1.91	0.52
1:D:271:PHE:HB3	1:D:291:LEU:HD13	1.91	0.52
1:C:57:SER:O	1:C:61:ILE:HG23	2.09	0.52
1:A:297:ASN:HA	4:A:501:D4G:N_2	2.25	0.52
1:D:143:ARG:HH11	1:D:143:ARG:HG3	1.75	0.52
1:D:360:GLN:HG2	5:D:523:HOH:O	2.08	0.52
1:B:351:TYR:O	1:B:355:VAL:HG23	2.10	0.52
1:B:37:PRO:HB2	1:B:48:GLN:NE2	2.25	0.52
1:B:97:GLU:HG3	5:B:2534:HOH:O	2.09	0.52
1:B:61:ILE:HD11	1:B:69:PHE:CE1	2.44	0.52
1:C:271:PHE:HB3	1:C:291:LEU:HD13	1.92	0.52
1:C:95:ALA:HB1	1:C:436:LYS:HD3	1.91	0.51
1:A:107:PHE:CE2	4:A:501:D4G:H10	2.46	0.51
1:B:409:GLN:CD	1:B:409:GLN:H	2.13	0.51
1:B:161:ARG:HH11	1:B:161:ARG:HG3	1.76	0.51
1:A:30:LYS:HG3	1:A:32:LYS:HB3	1.91	0.51
1:B:354:ALA:CB	1:B:417:LEU:HD13	2.41	0.51
1:C:453:PHE:O	1:C:457:MET:HG2	2.11	0.51
1:A:322:GLU:HG2	1:A:323:VAL:N	2.26	0.50
1:B:381:ARG:O	1:B:382:ASP:HB2	2.11	0.50
1:C:172:PHE:O	1:C:176:ARG:HG3	2.11	0.50
1:D:172:PHE:O	1:D:176:ARG:HG3	2.11	0.50
1:B:355:VAL:O	1:B:359:ILE:HG13	2.12	0.50
1:D:253:GLU:O	1:D:257:ARG:HG2	2.11	0.50
1:A:457:MET:CE	1:A:462:LEU:HD21	2.41	0.50
1:C:301:GLY:HA2	4:C:501:D4G:C5	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:ASP:OD1	1:D:337:LYS:HD3	2.11	0.50
1:B:92:VAL:HG23	1:B:434:ILE:HD12	1.94	0.49
1:D:352:MET:HE3	1:D:454:THR:HG22	1.93	0.49
1:B:354:ALA:HB2	1:B:417:LEU:HD13	1.94	0.49
1:A:84:HIS:HB2	1:A:398:VAL:HG13	1.95	0.49
1:B:59:MET:O	1:B:63:GLU:HG3	2.12	0.49
1:B:61:ILE:HD12	1:B:61:ILE:O	2.12	0.49
1:D:264:PRO:HG3	1:D:273:ILE:CD1	2.43	0.49
1:D:339:ARG:NH1	1:D:342:LYS:HE2	2.26	0.49
1:B:204:MET:O	1:B:208:ILE:HG12	2.12	0.49
1:C:476:LYS:HB2	1:C:485:ARG:HA	1.94	0.49
1:A:143:ARG:O	1:A:147:GLU:HG3	2.12	0.49
1:C:343:PHE:CE1	1:C:447:MET:HA	2.48	0.49
1:B:64:ARG:HD3	1:B:65:TYR:CE2	2.48	0.48
1:C:244:LEU:HD13	1:C:300:ILE:HD11	1.94	0.48
1:B:319:LYS:HD3	1:B:473:VAL:HG11	1.96	0.48
1:D:148:ARG:HH12	1:D:152:GLU:HB2	1.78	0.48
1:B:319:LYS:HD3	1:B:473:VAL:CG1	2.43	0.48
1:D:449:LEU:O	1:D:453:PHE:HB2	2.13	0.48
1:C:446:ARG:HG2	1:C:446:ARG:HH11	1.78	0.48
1:A:413:PRO:O	1:A:417:LEU:HD22	2.13	0.48
1:B:170:PRO:HB2	1:B:174:LEU:HD22	1.96	0.48
1:B:461:ARG:HB2	1:B:461:ARG:HH11	1.79	0.48
1:C:214:THR:HG23	1:C:217:GLY:H	1.79	0.48
1:B:494:ARG:NH1	1:B:494:ARG:HG3	2.29	0.48
1:D:131:SER:O	1:D:135:LEU:HB2	2.13	0.48
1:D:456:VAL:HG12	1:D:457:MET:CE	2.43	0.48
1:D:466:GLN:CG	1:D:471:ILE:HG12	2.44	0.47
1:B:89:GLU:CD	1:B:381:ARG:HH21	2.17	0.47
1:C:143:ARG:O	1:C:147:GLU:HG3	2.14	0.47
1:C:251:LYS:NZ	1:C:251:LYS:HB3	2.30	0.47
1:D:332:ASP:OD2	1:D:494:ARG:NH2	2.45	0.47
1:D:453:PHE:O	1:D:457:MET:HG2	2.13	0.47
1:C:352:MET:CE	1:C:454:THR:HG22	2.42	0.47
1:D:248:ILE:O	1:D:252:VAL:HG23	2.14	0.47
1:A:337:LYS:HD2	1:A:337:LYS:N	2.29	0.47
1:B:449:LEU:O	1:B:453:PHE:HB2	2.14	0.47
1:C:89:GLU:O	1:C:93:ASP:HB2	2.15	0.47
1:D:89:GLU:O	1:D:93:ASP:HB2	2.13	0.47
1:A:35:PRO:O	1:A:69:PHE:HB2	2.14	0.47
1:B:165:GLY:O	1:B:490:SER:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:MET:HG3	1:B:218:GLN:OE1	2.15	0.47
1:D:332:ASP:CG	1:D:494:ARG:HH22	2.17	0.47
1:B:123:ARG:HA	1:B:285:GLU:HG3	1.97	0.47
1:D:392:TYR:HB3	1:D:394:MET:HE1	1.96	0.47
1:A:272:LEU:O	1:A:276:GLN:HG3	2.14	0.47
1:A:466:GLN:HG2	5:A:2575:HOH:O	2.15	0.47
1:A:225:SER:HB2	1:D:225:SER:HB2	1.96	0.47
1:D:433:SER:HB3	3:D:500:HEM:HBA1	1.98	0.47
1:D:369:SER:HB2	1:D:395:LEU:HG	1.97	0.46
1:D:327:VAL:O	1:D:331:ILE:HG13	2.15	0.46
1:A:59:MET:O	1:A:63:GLU:HG3	2.15	0.46
1:D:96:GLU:OE1	1:D:436:LYS:NZ	2.49	0.46
1:C:213:SER:HA	1:C:479:GLY:HA3	1.97	0.46
1:D:476:LYS:HB2	1:D:485:ARG:HA	1.97	0.46
1:B:145:ILE:CD1	1:B:185:ILE:HD11	2.46	0.46
1:A:210:GLN:HE22	1:A:476:LYS:HZ3	1.64	0.46
1:A:442:GLU:O	1:A:446:ARG:HG3	2.15	0.46
1:B:64:ARG:HH11	1:B:64:ARG:HG2	1.81	0.46
1:C:344:GLU:HG3	5:C:551:HOH:O	2.16	0.45
1:D:354:ALA:HB2	1:D:417:LEU:HD13	1.98	0.45
1:B:53:GLN:HG3	1:B:56:ASN:HD22	1.81	0.45
1:A:301:GLY:HA2	4:A:501:D4G:C5	2.46	0.45
1:B:208:ILE:HD11	1:B:240:LEU:CB	2.39	0.45
1:C:358:GLU:CD	1:C:415:HIS:HD1	2.19	0.45
1:D:186:VAL:HG11	1:D:295:THR:HG23	1.98	0.45
1:D:271:PHE:CB	1:D:291:LEU:HD13	2.46	0.45
1:C:462:LEU:HD22	1:C:489:MET:HE1	1.97	0.45
1:D:260:ASP:O	1:D:262:ASN:N	2.50	0.45
1:D:145:ILE:HD13	1:D:185:ILE:HD11	1.99	0.45
1:A:449:LEU:O	1:A:453:PHE:HB2	2.16	0.45
1:C:186:VAL:HG11	1:C:295:THR:HG23	1.97	0.45
1:D:92:VAL:HG23	1:D:434:ILE:HD12	1.99	0.45
1:A:380:PHE:O	1:A:383:PHE:HB2	2.17	0.45
1:B:32:LYS:HE2	1:B:384:PHE:HB2	1.99	0.45
1:D:457:MET:CE	1:D:462:LEU:HD21	2.45	0.45
1:A:476:LYS:HE2	1:A:477:HIS:NE2	2.32	0.44
1:B:77:ARG:CG	1:B:77:ARG:NH1	2.77	0.44
1:D:352:MET:CE	1:D:454:THR:HG22	2.46	0.44
1:B:405:PHE:O	1:B:408:PRO:HD3	2.17	0.44
1:A:249:ALA:O	1:A:253:GLU:HG3	2.16	0.44
1:A:456:VAL:HG12	1:A:457:MET:CE	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:HIS:HB3	1:B:494:ARG:NH2	2.33	0.44
1:C:125:LYS:HZ1	1:C:129:ARG:HH12	1.65	0.44
1:B:101:ARG:HD3	1:B:117:VAL:O	2.18	0.44
1:B:324:GLU:OE2	1:B:462:LEU:HG	2.18	0.44
1:C:176:ARG:NH1	1:C:193:TYR:HB3	2.33	0.44
1:D:335:ILE:HG12	1:D:339:ARG:HH22	1.82	0.44
1:D:450:PHE:O	1:D:454:THR:HG23	2.18	0.44
1:B:208:ILE:HD12	1:B:241:LEU:HG	2.00	0.44
1:C:302:GLY:HA2	3:C:500:HEM:HMC2	2.00	0.44
1:A:30:LYS:C	1:A:32:LYS:H	2.21	0.44
1:B:40:LEU:HD11	1:D:47:LEU:HD21	1.99	0.44
1:B:352:MET:HG2	1:B:454:THR:HG22	2.00	0.44
1:C:143:ARG:CZ	1:C:147:GLU:HG2	2.48	0.44
1:A:110:VAL:HG11	1:A:241:LEU:HD22	2.00	0.43
1:B:168:ILE:O	1:B:488:THR:HA	2.18	0.43
1:C:168:ILE:O	1:C:168:ILE:HD12	2.18	0.43
1:B:145:ILE:HA	1:B:145:ILE:HD12	1.93	0.43
1:B:146:GLU:O	1:B:150:GLN:HG3	2.18	0.43
1:D:146:GLU:O	1:D:150:GLN:HG3	2.19	0.43
1:A:117:VAL:HG21	4:A:501:D4G:H8	1.99	0.43
1:D:271:PHE:CD2	1:D:291:LEU:HD13	2.54	0.43
1:D:152:GLU:HG3	1:D:177:THR:HG23	2.01	0.43
1:A:271:PHE:CB	1:A:291:LEU:HD13	2.47	0.43
1:B:258:THR:HG23	1:B:265:ARG:NH1	2.34	0.43
1:B:433:SER:CB	3:B:500:HEM:HBA1	2.48	0.43
1:D:337:LYS:HB3	1:D:337:LYS:HZ3	1.82	0.43
1:A:369:SER:HB2	1:A:395:LEU:HG	2.01	0.43
1:B:343:PHE:CE1	1:B:346:ARG:HD3	2.54	0.43
1:D:143:ARG:HG3	1:D:143:ARG:NH1	2.34	0.43
1:B:206:LEU:HA	1:B:206:LEU:HD12	1.90	0.43
1:B:467:SER:HB3	1:B:470:ASP:OD2	2.18	0.43
1:C:145:ILE:HD13	1:C:185:ILE:HD11	2.01	0.43
1:D:236:GLN:O	1:D:240:LEU:HG	2.19	0.43
1:A:271:PHE:CG	1:A:291:LEU:HD13	2.54	0.42
1:B:211:PHE:C	1:B:213:SER:H	2.22	0.42
1:C:168:ILE:C	1:C:168:ILE:HD12	2.39	0.42
1:B:462:LEU:HD22	1:B:489:MET:CE	2.49	0.42
1:A:30:LYS:CD	1:A:32:LYS:HB3	2.50	0.42
1:A:117:VAL:HG22	3:A:500:HEM:HAD1	2.01	0.42
1:C:322:GLU:HB2	5:C:710:HOH:O	2.20	0.42
1:C:375:LYS:O	1:C:387:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:LEU:HA	1:D:40:LEU:HD12	1.94	0.42
1:B:376:LYS:HA	1:B:387:LYS:CG	2.50	0.42
1:B:379:LYS:HE3	1:B:382:ASP:HA	2.01	0.42
1:C:343:PHE:O	1:C:346:ARG:HG2	2.19	0.42
1:C:418:ASN:OD1	1:C:419:GLU:N	2.53	0.42
1:D:326:LYS:HB3	1:D:351:TYR:CE2	2.55	0.42
1:D:115:GLY:O	1:D:119:SER:HB3	2.20	0.42
1:B:145:ILE:HD11	1:B:185:ILE:HD11	2.01	0.42
1:B:194:LYS:HD3	1:B:194:LYS:HA	1.86	0.42
1:B:327:VAL:HG13	1:B:352:MET:CE	2.49	0.42
1:B:52:GLU:HG2	1:B:52:GLU:O	2.18	0.42
1:C:433:SER:CB	3:C:500:HEM:HBA1	2.50	0.42
1:D:111:PHE:CE1	4:D:501:D4G:H9	2.55	0.42
1:A:88:ARG:HD3	5:A:2694:HOH:O	2.20	0.42
1:B:319:LYS:HG2	1:B:320:HIS:CE1	2.55	0.42
1:C:209:PHE:CG	1:C:304:GLU:HG2	2.55	0.42
1:B:129:ARG:HG3	1:B:129:ARG:HH11	1.84	0.42
1:B:161:ARG:HG3	5:B:2543:HOH:O	2.19	0.42
1:D:145:ILE:O	1:D:149:ILE:HG13	2.19	0.42
1:D:473:VAL:HG22	5:D:584:HOH:O	2.20	0.42
1:C:418:ASN:N	1:C:422:GLN:O	2.45	0.41
1:A:153:ALA:O	1:A:157:ILE:HG12	2.20	0.41
1:A:314:PHE:CE2	1:A:457:MET:HE1	2.56	0.41
1:B:195:ASP:OD1	1:B:197:GLU:N	2.45	0.41
1:B:202:LEU:HD22	1:B:206:LEU:HD22	2.01	0.41
1:A:376:LYS:O	1:A:377:ASP:C	2.58	0.41
1:B:301:GLY:HA2	4:B:501:D4G:C5	2.50	0.41
1:D:331:ILE:HG12	1:D:349:MET:CE	2.50	0.41
1:D:368:MET:HB3	1:D:394:MET:CE	2.50	0.41
1:B:205:MET:O	1:B:209:PHE:HD1	2.02	0.41
1:C:375:LYS:HE2	5:C:561:HOH:O	2.20	0.41
1:B:260:ASP:HA	1:B:261:PRO:HD2	1.88	0.41
1:C:417:LEU:HA	1:C:417:LEU:HD12	1.91	0.41
1:D:141:GLY:H	1:D:145:ILE:HG21	1.86	0.41
1:D:264:PRO:HG3	1:D:273:ILE:HD12	2.03	0.41
1:C:167:ASN:HD21	1:C:465:SER:HB3	1.85	0.41
1:D:33:LEU:HD11	1:D:77:ARG:CZ	2.50	0.41
1:A:358:GLU:OE1	1:A:358:GLU:HA	2.21	0.41
1:A:374:VAL:O	1:A:374:VAL:HG23	2.21	0.41
1:A:314:PHE:HE2	1:A:457:MET:CE	2.34	0.41
1:B:145:ILE:O	1:B:149:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:ALA:O	1:C:157:ILE:HG12	2.21	0.41
1:A:339:ARG:NH1	1:A:342:LYS:HZ2	2.19	0.41
1:B:318:MET:HE3	1:B:462:LEU:HB3	2.02	0.41
1:B:77:ARG:NH1	5:B:2537:HOH:O	2.53	0.41
1:A:126:GLN:HG3	1:A:286:PHE:CE2	2.57	0.41
1:B:101:ARG:CD	1:B:117:VAL:O	2.69	0.41
1:B:419:GLU:HG3	1:B:419:GLU:H	1.61	0.41
1:B:315:LEU:HD13	1:B:487:TYR:CD2	2.56	0.41
1:C:33:LEU:HD11	1:C:77:ARG:CZ	2.51	0.41
1:A:463:LYS:HB3	1:A:490:SER:HB2	2.02	0.40
1:B:274:ARG:NH1	1:B:286:PHE:CE2	2.89	0.40
1:D:257:ARG:HD3	1:D:257:ARG:N	2.36	0.40
1:B:259:LEU:HD12	1:B:260:ASP:H	1.86	0.40
3:D:500:HEM:NA	4:D:501:D4G:H2	2.35	0.40
1:D:117:VAL:HG22	3:D:500:HEM:HAD1	2.03	0.40
1:A:374:VAL:HG22	1:A:389:THR:N	2.36	0.40
1:B:186:VAL:HA	1:B:267:PHE:HB3	2.03	0.40
1:B:257:ARG:HG2	1:B:257:ARG:O	2.22	0.40
1:B:264:PRO:HG3	1:B:273:ILE:HD12	2.04	0.40
1:B:369:SER:HB2	1:B:395:LEU:HG	2.02	0.40
1:D:302:GLY:HA2	3:D:500:HEM:HMC2	2.03	0.40
1:A:416:PHE:O	1:A:417:LEU:HD13	2.22	0.40
1:A:433:SER:CB	3:A:500:HEM:HBA1	2.51	0.40
1:B:177:THR:HG23	5:B:2520:HOH:O	2.21	0.40
1:B:391:VAL:O	1:B:393:PRO:HD3	2.22	0.40
1:C:317:LEU:HD13	1:C:457:MET:CE	2.51	0.40
1:D:139:GLY:O	1:D:140:VAL:C	2.60	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	463/476 (97%)	444 (96%)	18 (4%)	1 (0%)	47	38
1	B	462/476 (97%)	438 (95%)	23 (5%)	1 (0%)	47	38
1	C	462/476 (97%)	450 (97%)	12 (3%)	0	100	100
1	D	462/476 (97%)	439 (95%)	21 (4%)	2 (0%)	34	22
All	All	1849/1904 (97%)	1771 (96%)	74 (4%)	4 (0%)	47	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	140	VAL
1	B	192	ASP
1	A	195	ASP
1	D	261	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	412/422 (98%)	404 (98%)	8 (2%)	57	50
1	B	412/422 (98%)	399 (97%)	13 (3%)	39	27
1	C	411/422 (97%)	400 (97%)	11 (3%)	44	34
1	D	411/422 (97%)	404 (98%)	7 (2%)	60	55
All	All	1646/1688 (98%)	1607 (98%)	39 (2%)	49	40

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	LEU
1	A	236	GLN
1	A	312	TYR
1	A	316	LEU
1	A	370	LEU
1	A	382	ASP
1	A	417	LEU

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Mol	Chain	Res	Type
1	A	453	PHE
1	B	53	GLN
1	B	61	ILE
1	B	77	ARG
1	B	135	LEU
1	B	174	LEU
1	B	195	ASP
1	B	202	LEU
1	B	234	GLN
1	B	312	TYR
1	B	417	LEU
1	B	419	GLU
1	B	453	PHE
1	B	486	ASN
1	C	40	LEU
1	C	61	ILE
1	C	96	GLU
1	C	135	LEU
1	C	143	ARG
1	C	146	GLU
1	C	148	ARG
1	C	236	GLN
1	C	312	TYR
1	C	414	GLN
1	C	417	LEU
1	D	40	LEU
1	D	174	LEU
1	D	210	GLN
1	D	234	GLN
1	D	312	TYR
1	D	337	LYS
1	D	417	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	126	GLN
1	A	210	GLN
1	B	56	ASN
1	B	320	HIS
1	B	409	GLN

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Mol	Chain	Res	Type
1	B	412	ASN
1	B	414	GLN
1	B	466	GLN
1	C	409	GLN
1	C	414	GLN
1	D	256	GLN
1	D	276	GLN
1	D	340	GLN
1	D	409	GLN
1	D	418	ASN

### 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 ⓘ

11 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	HEM	A	500	1,4	27,50,50	1.88	7 (25%)	17,82,82	1.52	3 (17%)
3	HEM	B	500	1,4	27,50,50	1.92	10 (37%)	17,82,82	1.81	4 (23%)
2	SO4	A	2502	-	4,4,4	0.29	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	B	2504	-	4,4,4	0.28	0	6,6,6	0.08	0
4	D4G	D	501	3	15,15,15	1.94	6 (40%)	18,18,18	1.91	6 (33%)
4	D4G	B	501	3	15,15,15	1.93	6 (40%)	18,18,18	1.95	8 (44%)
4	D4G	C	501	3	15,15,15	1.92	7 (46%)	18,18,18	1.95	8 (44%)
4	D4G	A	501	3	15,15,15	1.94	6 (40%)	18,18,18	1.94	7 (38%)
3	HEM	D	500	1,4	27,50,50	1.92	6 (22%)	17,82,82	1.71	4 (23%)
2	SO4	A	2503	-	4,4,4	0.27	0	6,6,6	0.08	0
3	HEM	C	500	1,4	27,50,50	1.87	8 (29%)	17,82,82	1.69	5 (29%)

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	HEM	A	500	1,4	-	0/6/54/54	-
3	HEM	B	500	1,4	-	0/6/54/54	-
4	D4G	A	501	3	-	3/5/5/5	0/2/2/2
4	D4G	D	501	3	-	2/5/5/5	0/2/2/2
4	D4G	B	501	3	-	2/5/5/5	0/2/2/2
4	D4G	C	501	3	-	0/5/5/5	0/2/2/2
3	HEM	D	500	1,4	-	0/6/54/54	-
3	HEM	C	500	1,4	-	0/6/54/54	-

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	HEM	C3C-CAC	-5.14	1.37	1.47
3	D	500	HEM	C3C-CAC	-4.84	1.37	1.47
3	C	500	HEM	C3C-CAC	-4.81	1.37	1.47
3	B	500	HEM	C3C-CAC	-4.60	1.38	1.47
3	D	500	HEM	CMA-C3A	3.49	1.58	1.51
3	A	500	HEM	C1D-ND	-3.16	1.29	1.36
3	B	500	HEM	CMA-C3A	3.10	1.58	1.51
4	B	501	D4G	C4-S_1	-3.04	1.73	1.78
3	D	500	HEM	CBB-CAB	3.03	1.49	1.29
3	A	500	HEM	CMA-C3A	2.99	1.57	1.51
3	C	500	HEM	CMA-C3A	2.99	1.57	1.51
3	B	500	HEM	CBB-CAB	2.96	1.48	1.29
4	B	501	D4G	C7-C6	2.96	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	501	D4G	C7-C6	2.93	1.44	1.39
3	D	500	HEM	C1D-ND	-2.90	1.30	1.36
4	D	501	D4G	C7-C6	2.87	1.44	1.39
3	A	500	HEM	CBB-CAB	2.86	1.48	1.29
4	D	501	D4G	C5-C1	2.85	1.44	1.38
3	C	500	HEM	CBB-CAB	2.84	1.48	1.29
3	B	500	HEM	C1D-ND	-2.82	1.30	1.36
4	A	501	D4G	C4-S_1	-2.79	1.73	1.78
4	A	501	D4G	C7-C6	2.77	1.44	1.39
3	C	500	HEM	C1D-ND	-2.76	1.30	1.36
4	A	501	D4G	C5-C1	2.65	1.43	1.38
3	D	500	HEM	CAD-C3D	2.59	1.56	1.52
3	A	500	HEM	CMC-C2C	2.56	1.57	1.51
4	C	501	D4G	C10-C6	2.53	1.44	1.39
4	B	501	D4G	C10-C6	2.51	1.44	1.39
3	C	500	HEM	CAD-C3D	2.48	1.56	1.52
4	A	501	D4G	C5-C4	2.47	1.44	1.39
3	B	500	HEM	CAD-C3D	2.47	1.56	1.52
3	B	500	HEM	CMC-C2C	2.45	1.57	1.51
4	D	501	D4G	C10-C6	2.44	1.44	1.39
4	C	501	D4G	C5-C4	2.41	1.43	1.39
4	A	501	D4G	C10-C6	2.39	1.43	1.39
4	C	501	D4G	C5-C1	2.37	1.43	1.38
3	C	500	HEM	C3B-CAB	-2.36	1.43	1.47
3	C	500	HEM	CMC-C2C	2.35	1.57	1.51
3	B	500	HEM	C3B-C2B	2.32	1.43	1.40
3	A	500	HEM	CAD-C3D	2.31	1.56	1.52
4	D	501	D4G	C5-C4	2.29	1.43	1.39
4	B	501	D4G	C7-C8	2.27	1.43	1.38
3	B	500	HEM	CAA-C2A	2.27	1.55	1.52
4	D	501	D4G	C3-C4	2.26	1.43	1.39
4	B	501	D4G	C3-C4	2.24	1.43	1.39
3	D	500	HEM	CMC-C2C	2.21	1.56	1.51
4	C	501	D4G	C4-S_1	-2.18	1.74	1.78
3	C	500	HEM	C4A-NA	-2.17	1.31	1.36
4	C	501	D4G	C7-C8	2.15	1.42	1.38
3	B	500	HEM	C3B-CAB	-2.09	1.43	1.47
4	A	501	D4G	C7-C8	2.09	1.42	1.38
4	C	501	D4G	C3-C4	2.09	1.43	1.39
4	D	501	D4G	C4-S_1	-2.06	1.74	1.78
3	B	500	HEM	C1C-C2C	-2.02	1.38	1.42
3	A	500	HEM	C3B-CAB	-2.02	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	D4G	C10-C9	2.00	1.42	1.38

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	501	D4G	C9-N_2-C8	3.65	125.43	116.85
4	B	501	D4G	C1-N_1-C2	3.59	125.29	116.85
3	B	500	HEM	CAD-CBD-CGD	3.58	118.67	112.67
4	A	501	D4G	C9-N_2-C8	3.57	125.25	116.85
4	C	501	D4G	C9-N_2-C8	3.57	125.24	116.85
4	C	501	D4G	C1-N_1-C2	3.52	125.13	116.85
4	A	501	D4G	C1-N_1-C2	3.52	125.12	116.85
4	B	501	D4G	C9-N_2-C8	3.48	125.03	116.85
4	D	501	D4G	C1-N_1-C2	3.43	124.93	116.85
3	B	500	HEM	CMB-C2B-C3B	3.26	130.78	124.68
3	B	500	HEM	C4C-C3C-C2C	-3.21	104.65	106.90
3	D	500	HEM	CMB-C2B-C3B	3.21	130.69	124.68
3	C	500	HEM	CMB-C2B-C3B	3.16	130.58	124.68
4	A	501	D4G	C5-C1-N_1	-3.07	118.28	123.62
3	C	500	HEM	C4C-C3C-C2C	-3.02	104.79	106.90
3	D	500	HEM	C4C-C3C-C2C	-2.93	104.85	106.90
4	C	501	D4G	C5-C1-N_1	-2.92	118.54	123.62
3	D	500	HEM	CAD-CBD-CGD	2.89	117.53	112.67
3	A	500	HEM	CMB-C2B-C3B	2.78	129.89	124.68
4	D	501	D4G	C5-C1-N_1	-2.78	118.77	123.62
4	A	501	D4G	C10-C9-N_2	-2.78	118.78	123.62
4	C	501	D4G	C10-C9-N_2	-2.76	118.81	123.62
4	D	501	D4G	C7-C8-N_2	-2.76	118.82	123.62
3	C	500	HEM	CAD-CBD-CGD	2.75	117.28	112.67
4	B	501	D4G	C5-C1-N_1	-2.74	118.84	123.62
4	B	501	D4G	C10-C9-N_2	-2.71	118.91	123.62
4	D	501	D4G	C10-C9-N_2	-2.70	118.92	123.62
4	A	501	D4G	C7-C8-N_2	-2.69	118.94	123.62
3	A	500	HEM	C4C-C3C-C2C	-2.68	105.02	106.90
4	C	501	D4G	C7-C8-N_2	-2.68	118.95	123.62
4	B	501	D4G	C3-C2-N_1	-2.65	119.00	123.62
4	B	501	D4G	C7-C8-N_2	-2.62	119.05	123.62
3	A	500	HEM	CAD-CBD-CGD	2.56	116.96	112.67
3	D	500	HEM	CAA-CBA-CGA	2.48	116.83	112.67
4	C	501	D4G	C3-C2-N_1	-2.44	119.38	123.62
3	B	500	HEM	CAA-CBA-CGA	2.42	116.73	112.67
4	D	501	D4G	C3-C2-N_1	-2.40	119.44	123.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	D4G	C6-S_2-S_1	2.27	110.91	104.90
4	A	501	D4G	C3-C2-N_1	-2.25	119.71	123.62
4	B	501	D4G	C5-C4-C3	2.22	122.53	118.82
4	A	501	D4G	C5-C4-C3	2.14	122.40	118.82
4	B	501	D4G	C6-S_2-S_1	2.12	110.53	104.90
3	C	500	HEM	CMA-C3A-C4A	-2.05	125.31	128.46
3	C	500	HEM	CAA-CBA-CGA	2.03	116.08	112.67
4	C	501	D4G	C5-C4-C3	2.02	122.21	118.82

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	D4G	C7-C6-S_2-S_1
4	A	501	D4G	C10-C6-S_2-S_1
4	D	501	D4G	C10-C6-S_2-S_1
4	D	501	D4G	C7-C6-S_2-S_1
4	B	501	D4G	C10-C6-S_2-S_1
4	A	501	D4G	C5-C4-S_1-S_2
4	B	501	D4G	C7-C6-S_2-S_1

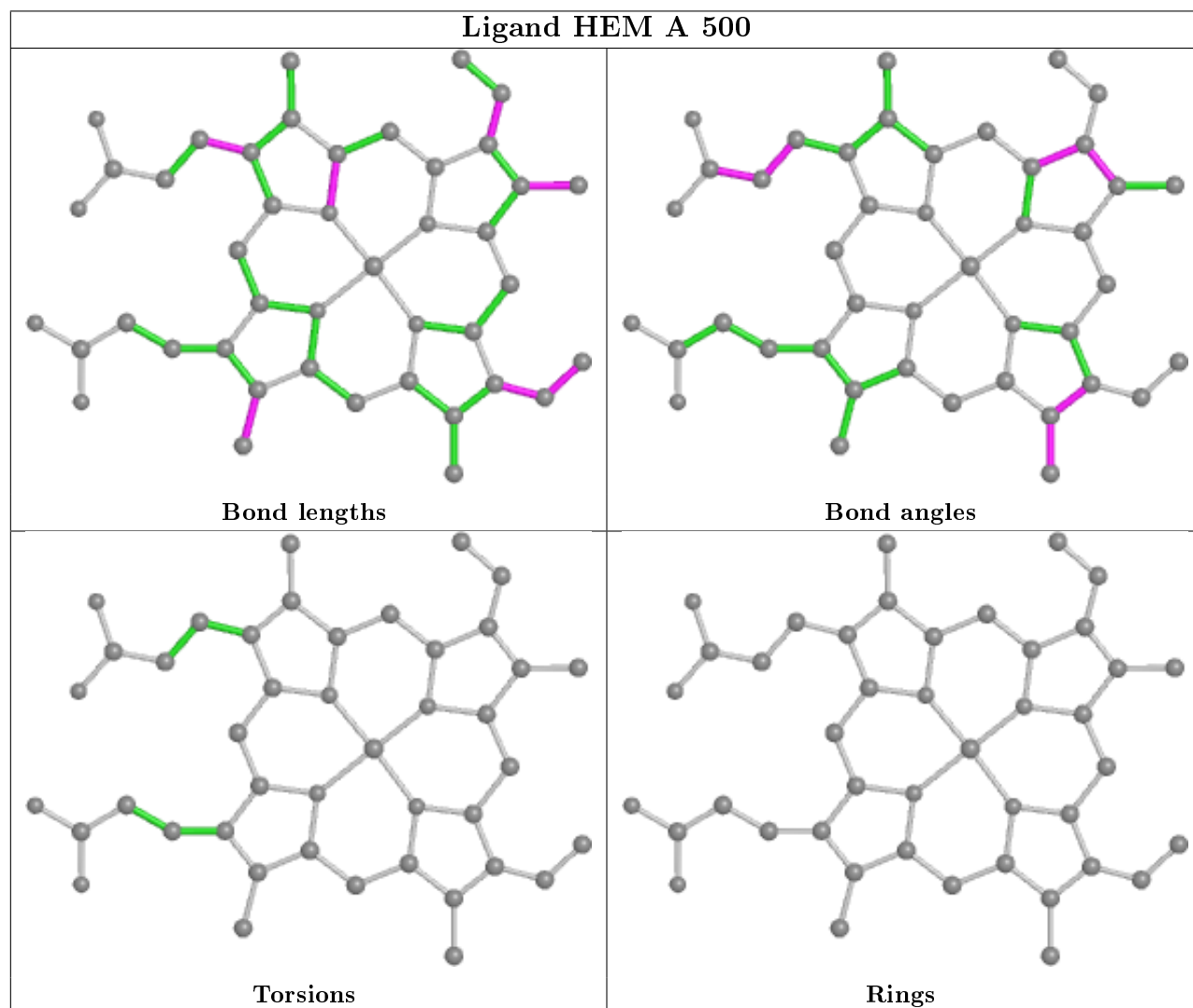
There are no ring outliers.

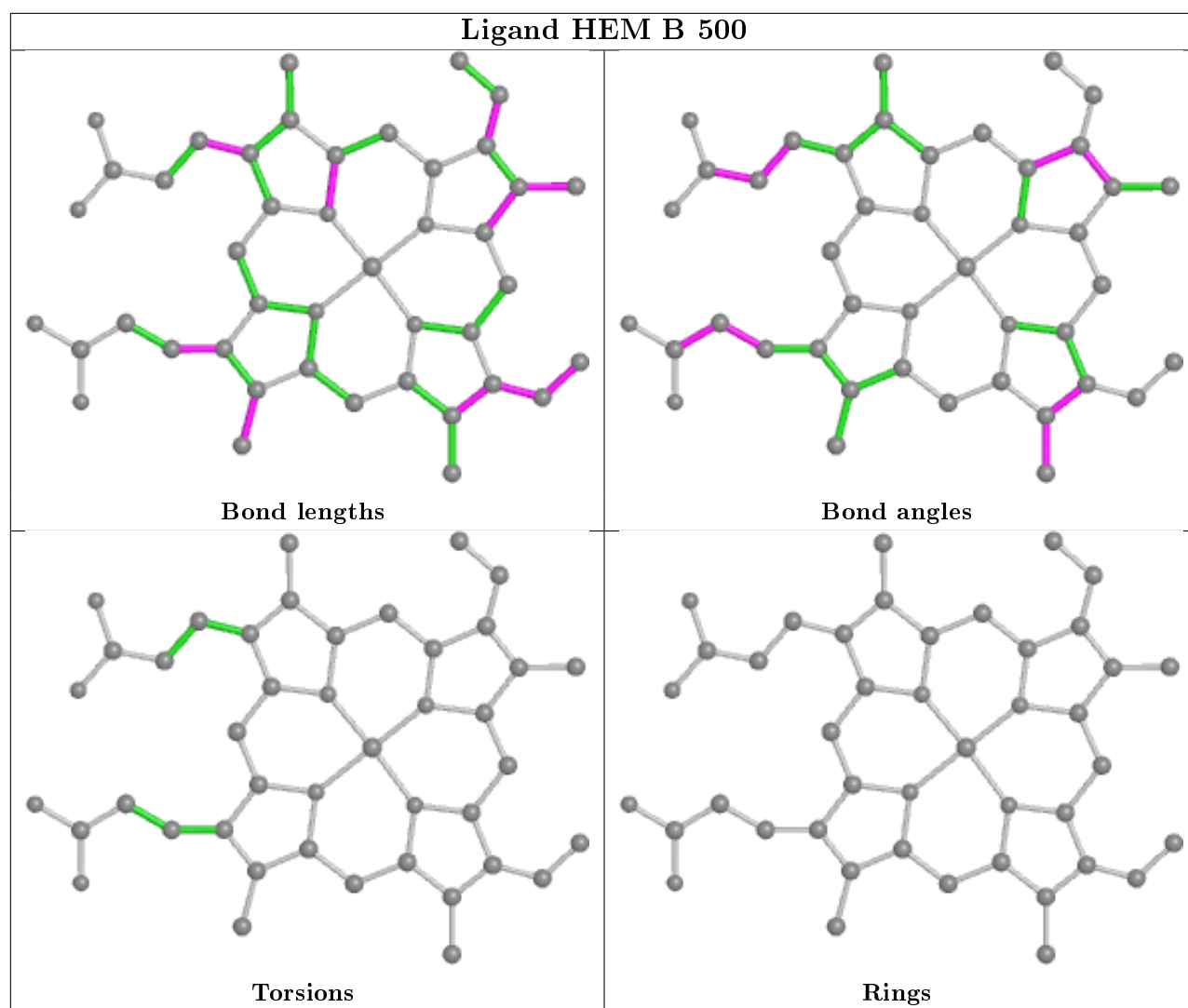
8 monomers are involved in 21 short contacts:

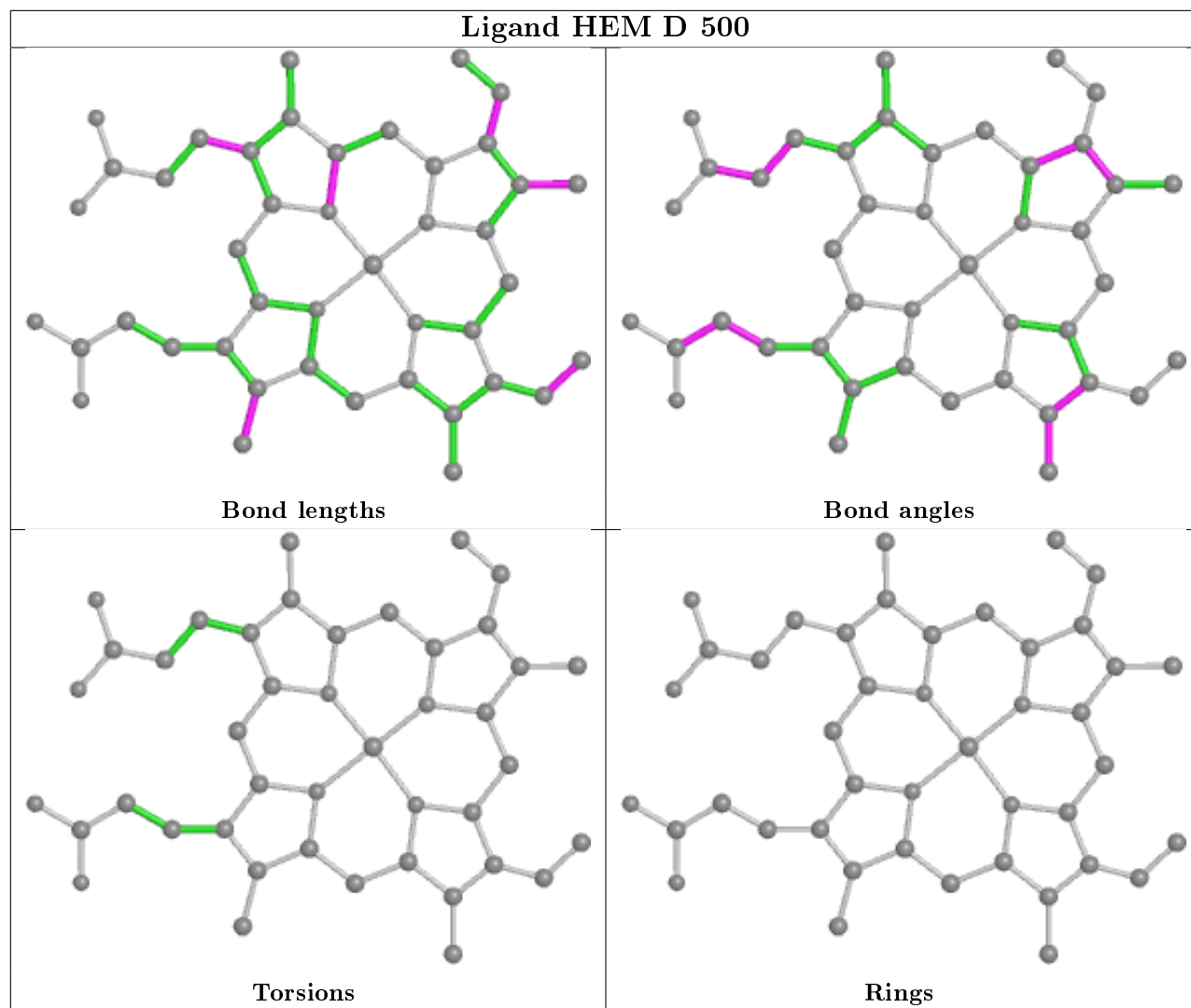
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	HEM	3	0
3	B	500	HEM	2	0
4	D	501	D4G	3	0
4	B	501	D4G	1	0
4	C	501	D4G	1	0
4	A	501	D4G	4	0
3	D	500	HEM	4	0
3	C	500	HEM	4	0

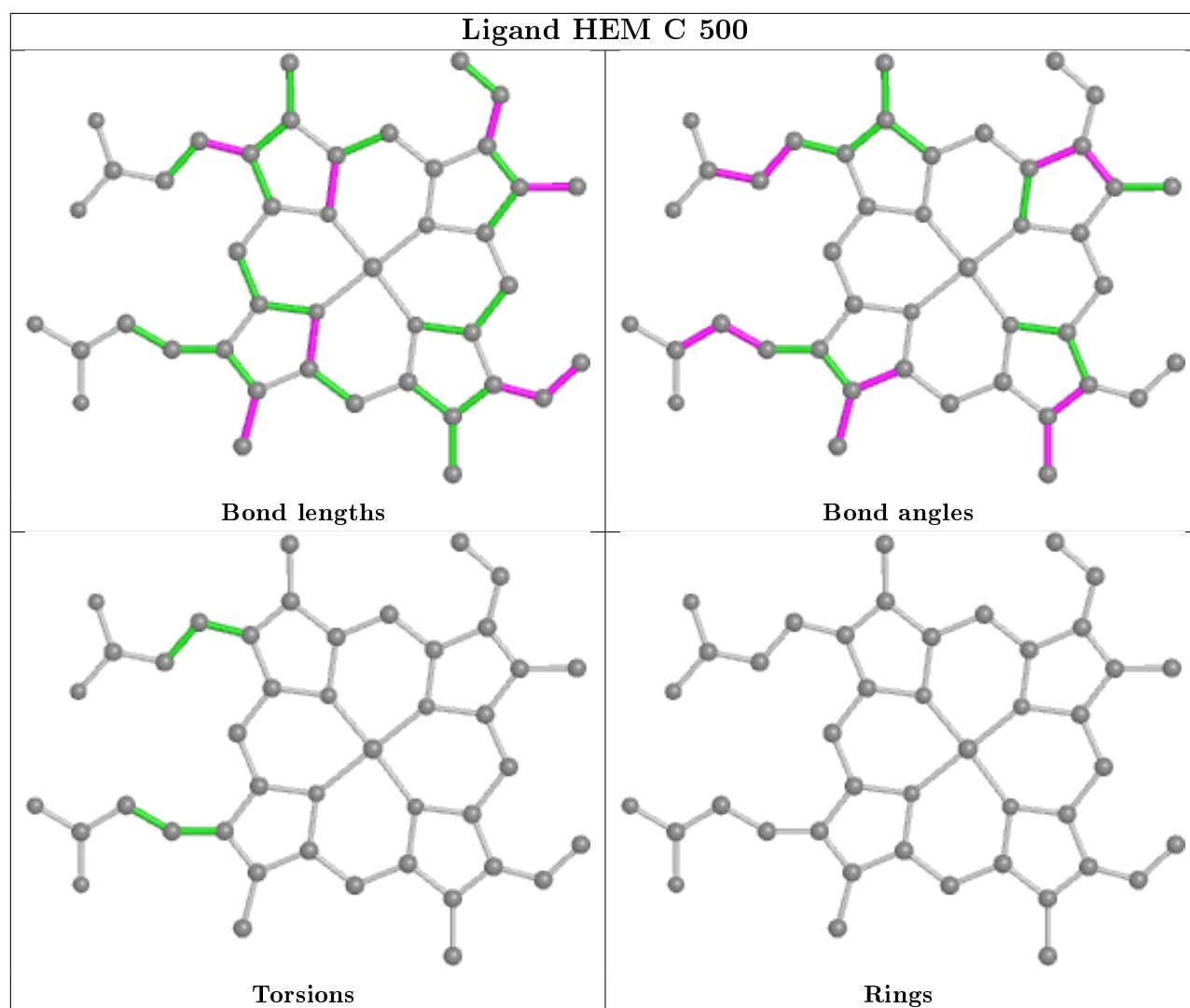
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	465/476 (97%)	1.05	42 (9%) 9 15	14, 26, 44, 64	0
1	B	464/476 (97%)	1.25	73 (15%) 2 3	16, 33, 51, 71	0
1	C	464/476 (97%)	1.02	46 (9%) 7 12	13, 25, 42, 51	0
1	D	464/476 (97%)	1.15	76 (16%) 1 2	14, 27, 54, 68	0
All	All	1857/1904 (97%)	1.12	237 (12%) 3 6	13, 28, 48, 71	0

All (237) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	495	HIS	8.6
1	B	193	TYR	6.0
1	A	61	ILE	5.8
1	D	261	PRO	5.7
1	D	264	PRO	5.3
1	D	143	ARG	5.2
1	A	30	LYS	4.6
1	B	323	VAL	4.6
1	C	417	LEU	4.2
1	B	189	ASP	4.2
1	D	138	PHE	4.1
1	D	355	VAL	4.1
1	B	384	PHE	4.1
1	D	276	GLN	4.1
1	D	144	GLY	4.0
1	B	325	ALA	3.9
1	A	249	ALA	3.8
1	A	32	LYS	3.8
1	A	268	ILE	3.8
1	D	334	VAL	3.8
1	D	273	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	417	LEU	3.7
1	C	31	GLY	3.6
1	C	391	VAL	3.6
1	D	78	VAL	3.6
1	D	140	VAL	3.6
1	B	379	LYS	3.5
1	D	379	LYS	3.5
1	B	405	PHE	3.5
1	D	141	GLY	3.5
1	C	451	LEU	3.5
1	C	384	PHE	3.4
1	B	143	ARG	3.4
1	A	384	PHE	3.4
1	B	33	LEU	3.4
1	C	327	VAL	3.3
1	D	31	GLY	3.3
1	B	482	THR	3.3
1	D	280	LYS	3.3
1	A	33	LEU	3.2
1	C	420	LYS	3.2
1	C	149	ILE	3.2
1	A	379	LYS	3.1
1	B	259	LEU	3.1
1	D	277	GLU	3.1
1	B	194	LYS	3.1
1	D	456	VAL	3.1
1	A	287	TYR	3.1
1	B	411	PHE	3.1
1	B	469	LYS	3.1
1	D	336	GLY	3.1
1	D	331	ILE	3.0
1	D	274	ARG	3.0
1	D	139	GLY	3.0
1	B	380	PHE	3.0
1	A	155	PHE	3.0
1	D	335	ILE	2.9
1	D	302	GLY	2.9
1	A	230	LEU	2.9
1	B	494	ARG	2.9
1	B	480	PHE	2.9
1	D	194	LYS	2.9
1	C	365	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	492	LEU	2.9
1	B	336	GLY	2.8
1	C	418	ASN	2.8
1	A	359	ILE	2.8
1	D	279	GLU	2.8
1	B	483	ILE	2.8
1	B	70	THR	2.8
1	A	483	ILE	2.8
1	D	259	LEU	2.7
1	B	257	ARG	2.7
1	D	136	ARG	2.7
1	D	135	LEU	2.7
1	B	64	ARG	2.7
1	A	383	PHE	2.7
1	A	465	SER	2.7
1	D	278	GLU	2.7
1	C	370	LEU	2.6
1	D	445	ALA	2.6
1	D	284	THR	2.6
1	A	238	PHE	2.6
1	D	460	PHE	2.6
1	A	291	LEU	2.6
1	B	465	SER	2.6
1	B	343	PHE	2.6
1	A	258	THR	2.6
1	D	430	VAL	2.6
1	B	464	SER	2.5
1	A	306	VAL	2.5
1	D	339	ARG	2.5
1	C	409	GLN	2.5
1	B	196	LYS	2.5
1	D	288	LEU	2.5
1	B	61	ILE	2.5
1	B	292	VAL	2.5
1	B	374	VAL	2.5
1	C	138	PHE	2.5
1	D	370	LEU	2.5
1	B	53	GLN	2.5
1	B	467	SER	2.5
1	B	473	VAL	2.5
1	D	115	GLY	2.5
1	B	493	PRO	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	479	GLY	2.4
1	D	420	LYS	2.4
1	C	273	ILE	2.4
1	D	129	ARG	2.4
1	B	312	TYR	2.4
1	C	491	PHE	2.4
1	D	198	PHE	2.4
1	D	450	PHE	2.4
1	A	282	PRO	2.4
1	C	105	ALA	2.4
1	C	445	ALA	2.4
1	B	419	GLU	2.4
1	A	382	ASP	2.4
1	C	472	ASP	2.4
1	A	219	LEU	2.4
1	B	383	PHE	2.4
1	D	452	PHE	2.4
1	B	125	LYS	2.4
1	B	461	ARG	2.4
1	B	471	ILE	2.4
1	B	256	GLN	2.4
1	B	276	GLN	2.4
1	C	287	TYR	2.4
1	C	262	ASN	2.4
1	B	478	VAL	2.4
1	B	382	ASP	2.3
1	A	272	LEU	2.3
1	D	257	ARG	2.3
1	D	444	LEU	2.3
1	C	369	SER	2.3
1	D	185	ILE	2.3
1	D	325	ALA	2.3
1	A	70	THR	2.3
1	B	209	PHE	2.3
1	B	287	TYR	2.3
1	C	431	PRO	2.3
1	C	178	VAL	2.3
1	C	300	ILE	2.3
1	C	306	VAL	2.3
1	D	92	VAL	2.3
1	C	481	ALA	2.3
1	D	142	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	252	VAL	2.3
1	B	246	ASP	2.3
1	D	145	ILE	2.3
1	C	350	PRO	2.3
1	D	468	PRO	2.3
1	C	298	LEU	2.3
1	D	423	PHE	2.3
1	A	463	LYS	2.3
1	C	334	VAL	2.3
1	D	327	VAL	2.3
1	B	208	ILE	2.3
1	D	350	PRO	2.3
1	D	81	LEU	2.3
1	B	314	PHE	2.2
1	A	330	GLU	2.2
1	B	484	PRO	2.2
1	C	398	VAL	2.2
1	A	31	GLY	2.2
1	A	336	GLY	2.2
1	C	194	LYS	2.2
1	D	271	PHE	2.2
1	D	178	VAL	2.2
1	D	196	LYS	2.2
1	D	35	PRO	2.2
1	A	467	SER	2.2
1	D	286	PHE	2.2
1	D	308	THR	2.2
1	A	335	ILE	2.2
1	D	332	ASP	2.2
1	B	170	PRO	2.2
1	A	462	LEU	2.2
1	D	417	LEU	2.2
1	B	212	THR	2.2
1	B	421	GLY	2.2
1	A	69	PHE	2.2
1	C	107	PHE	2.2
1	B	407	ASN	2.1
1	D	109	TRP	2.1
1	D	424	LYS	2.1
1	B	69	PHE	2.1
1	B	491	PHE	2.1
1	A	373	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	366	ILE	2.1
1	A	376	LYS	2.1
1	A	378	THR	2.1
1	B	300	ILE	2.1
1	C	259	LEU	2.1
1	C	395	LEU	2.1
1	A	60	LYS	2.1
1	D	366	ILE	2.1
1	C	462	LEU	2.1
1	D	371	ALA	2.1
1	B	337	LYS	2.1
1	B	476	LYS	2.1
1	C	261	PRO	2.1
1	D	283	ASN	2.1
1	B	98	PHE	2.1
1	B	213	SER	2.1
1	B	315	LEU	2.1
1	C	333	ARG	2.1
1	C	69	PHE	2.1
1	D	391	VAL	2.1
1	A	434	ILE	2.1
1	C	61	ILE	2.1
1	B	439	CYS	2.1
1	B	492	LEU	2.1
1	C	219	LEU	2.1
1	C	272	LEU	2.1
1	B	107	PHE	2.0
1	C	209	PHE	2.0
1	D	254	HIS	2.0
1	B	335	ILE	2.0
1	C	241	LEU	2.0
1	D	268	ILE	2.0
1	C	454	THR	2.0
1	D	275	MET	2.0
1	D	418	ASN	2.0
1	B	60	LYS	2.0
1	A	261	PRO	2.0
1	A	365	VAL	2.0
1	B	413	PRO	2.0
1	B	423	PHE	2.0
1	D	384	PHE	2.0
1	A	91	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	73	LEU	2.0
1	C	366	ILE	2.0
1	C	444	LEU	2.0
1	D	199	LEU	2.0
1	B	215	SER	2.0
1	A	257	ARG	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 [i](#)

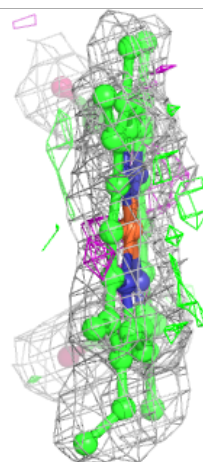
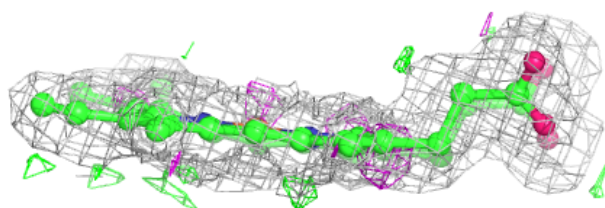
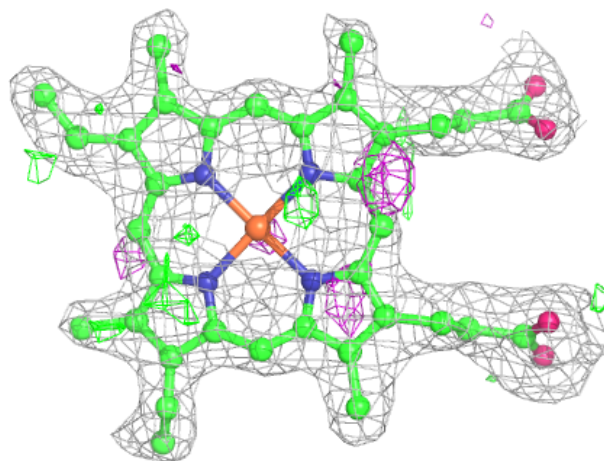
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	D4G	D	501	14/14	0.75	0.29	35,43,48,50	0
4	D4G	A	501	14/14	0.75	0.25	28,42,52,52	0
2	SO4	A	2502	5/5	0.78	0.21	66,66,66,67	0
4	D4G	C	501	14/14	0.81	0.20	28,42,46,49	0
4	D4G	B	501	14/14	0.81	0.19	26,40,46,48	0
2	SO4	B	2504	5/5	0.87	0.13	63,64,64,64	0
3	HEM	B	500	43/43	0.94	0.16	16,20,24,28	0
3	HEM	D	500	43/43	0.94	0.21	18,21,23,25	0
3	HEM	C	500	43/43	0.94	0.21	15,19,22,26	0
3	HEM	A	500	43/43	0.95	0.17	12,17,20,22	0
2	SO4	A	2503	5/5	0.96	0.13	31,33,33,34	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.

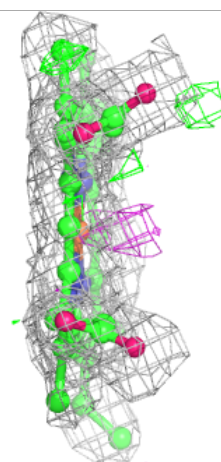
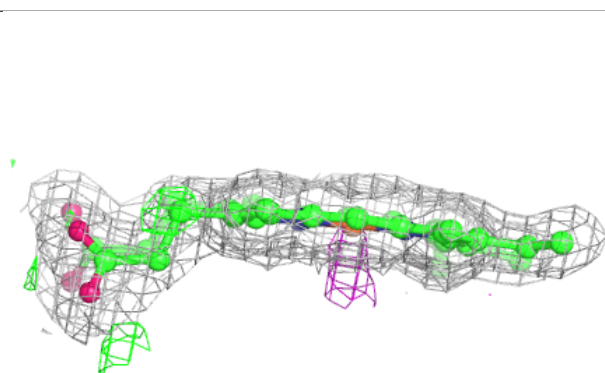
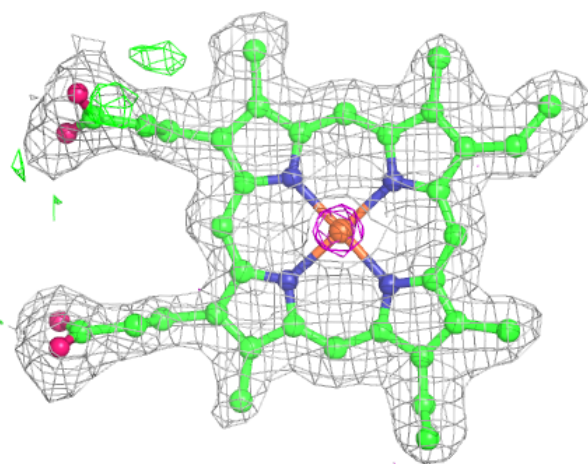
**Electron density around HEM B 500:**

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



**Electron density around HEM D 500:**

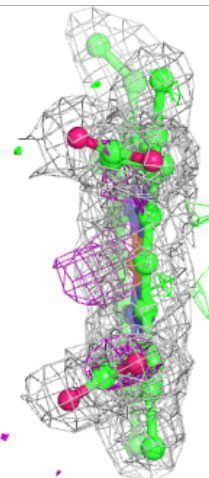
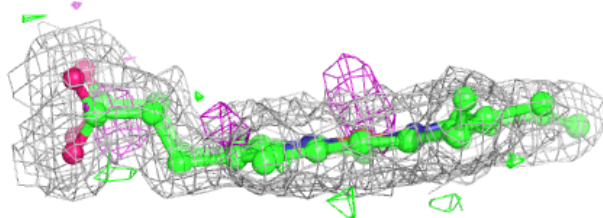
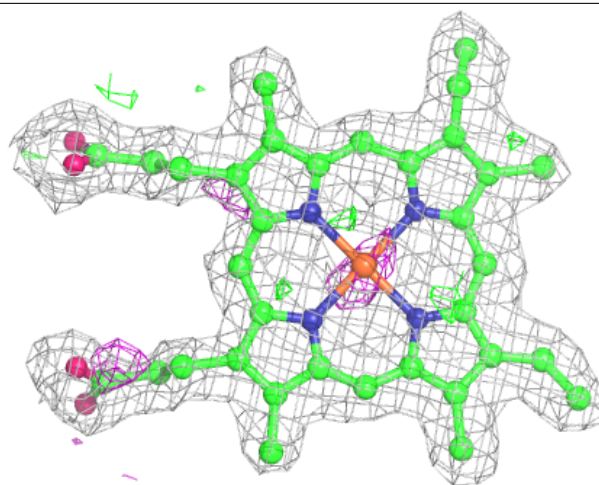
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

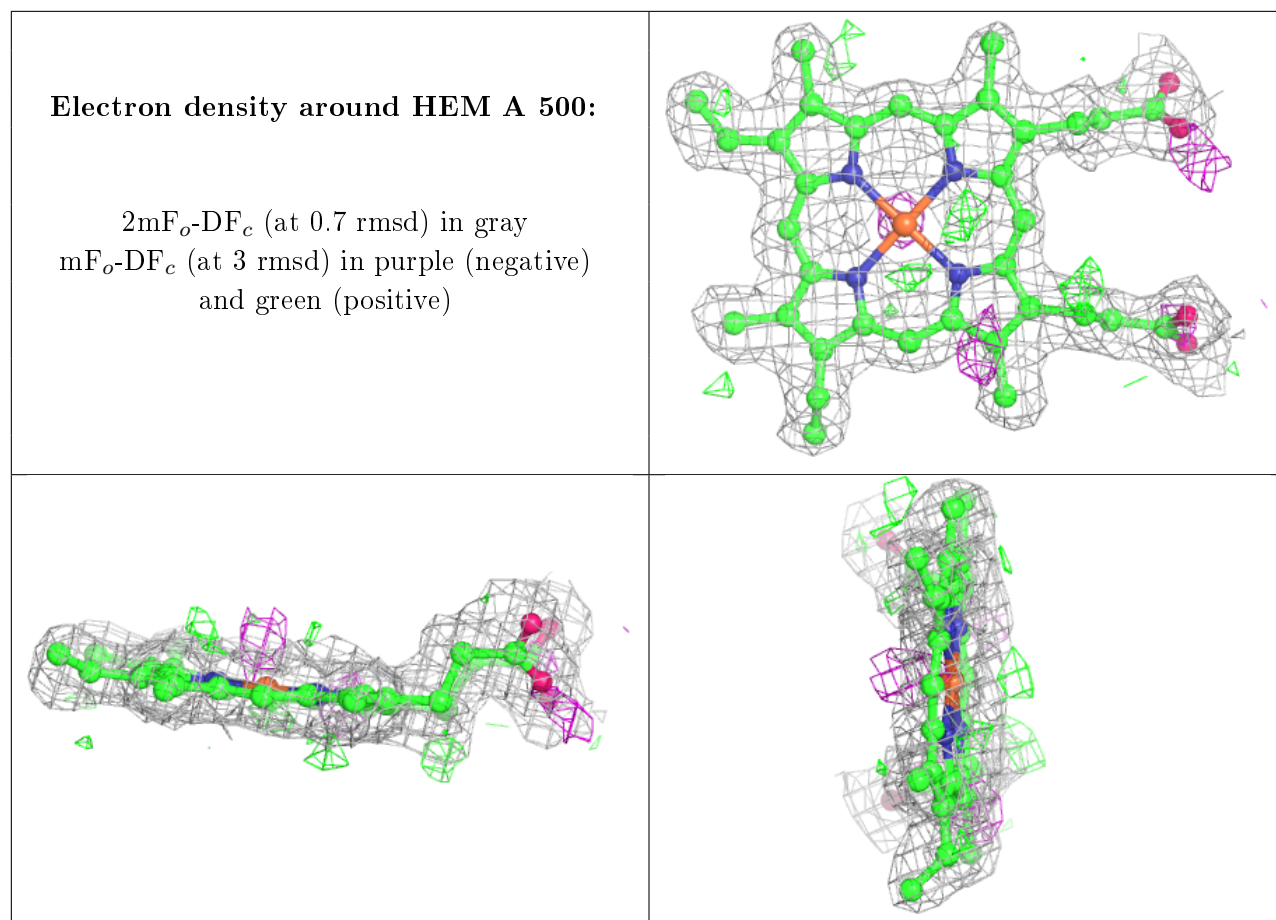




**Electron density around HEM C 500:**

$2mF_o-DF_c$  (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.