



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 11:44 AM UTC

PDB ID : 2FDU / pdb_00002fdu
Title : Microsomal P450 2A6 with the inhibitor N,N-Dimethyl(5-(pyridin-3-yl)furan-2-yl)methanamine bound
Authors : Yano, J.K.; Stout, C.D.; Johnson, E.F.
Deposited on : 2005-12-14
Resolution : 1.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

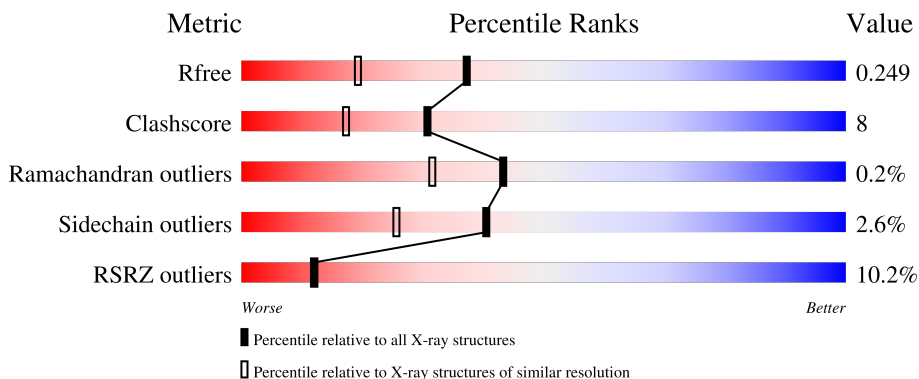
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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

Mol	Chain	Length	Quality of chain
1	A	476	
1	B	476	
1	C	476	
1	D	476	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16510 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome P450 2A6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	465	3760	2414	650	678	18	0	0	0
1	B	463	3747	2406	647	676	18	0	0	0
1	C	464	3751	2408	648	677	18	0	0	0
1	D	464	3751	2408	648	677	18	0	0	0

There are 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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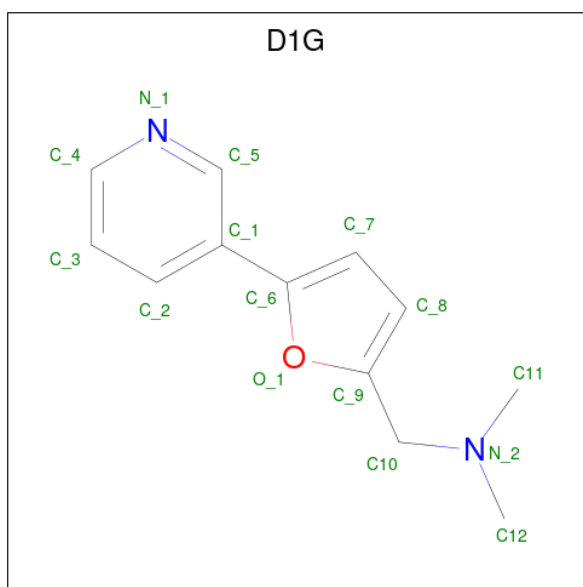
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Chain	Residue	Modelled	Actual	Comment	Reference
C	24	ALA	-	cloning artifact	UNP P11509
C	25	LYS	-	cloning artifact	UNP P11509
C	26	LYS	-	cloning artifact	UNP P11509
C	27	THR	-	cloning artifact	UNP P11509
C	28	SER	-	cloning artifact	UNP P11509
C	495	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 (CCD ID: SO4) (formula: O₄S).



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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	12	2	1		
4	B	1	Total	C	N	O	0	0
			15	12	2	1		
4	C	1	Total	C	N	O	0	0
			15	12	2	1		
4	D	1	Total	C	N	O	0	0
			15	12	2	1		

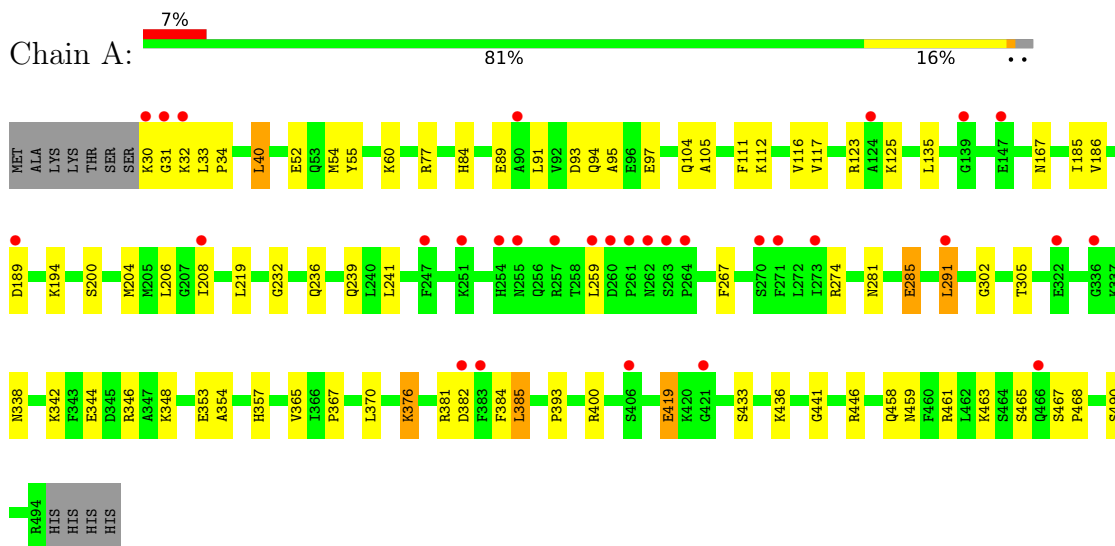
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	346	Total	O	0	0
			346	346		
5	B	228	Total	O	0	0
			228	228		
5	C	368	Total	O	0	0
			368	368		
5	D	317	Total	O	0	0
			317	317		

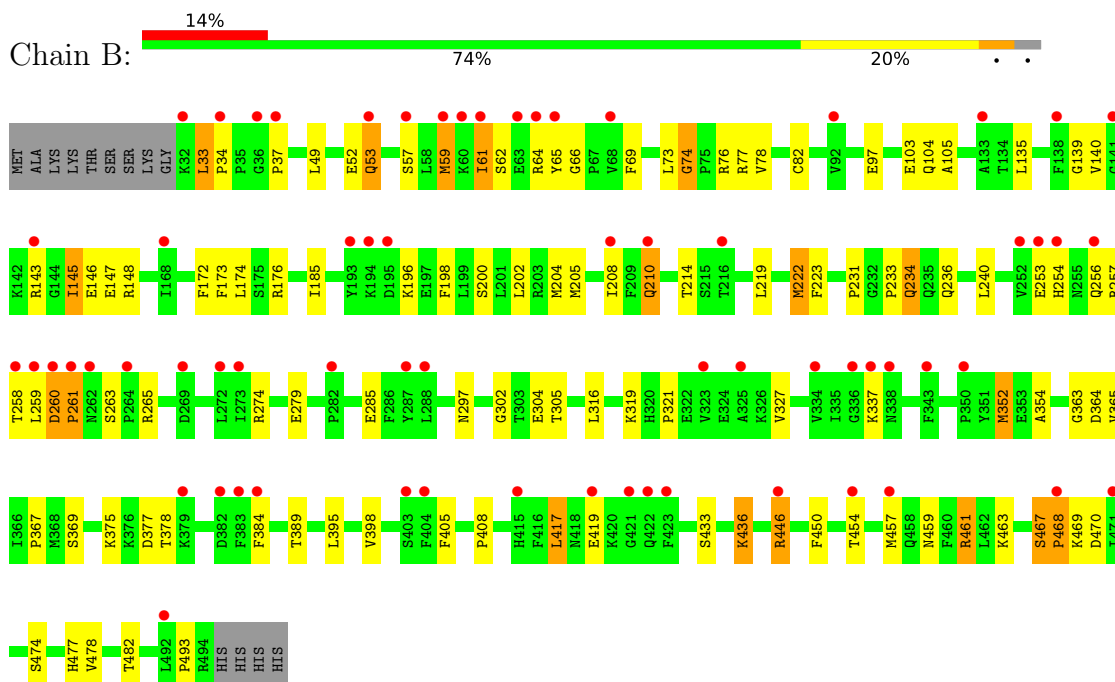
3 Residue-property plots i

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

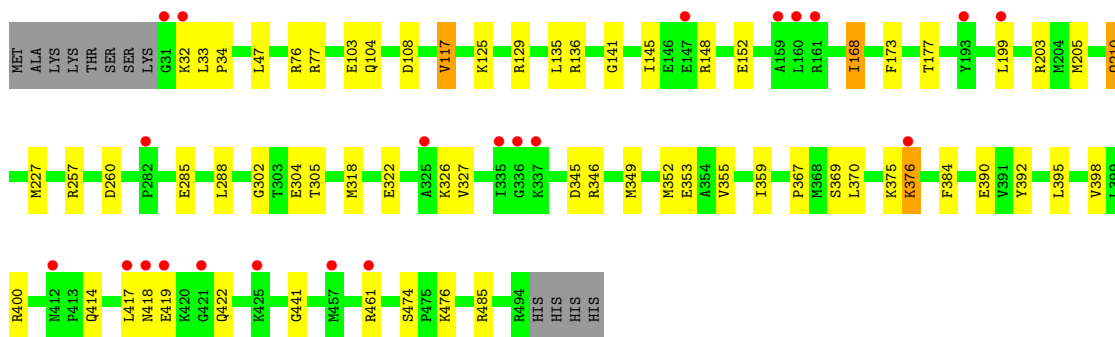
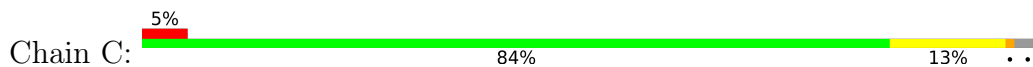
• Molecule 1: Cytochrome P450 2A6



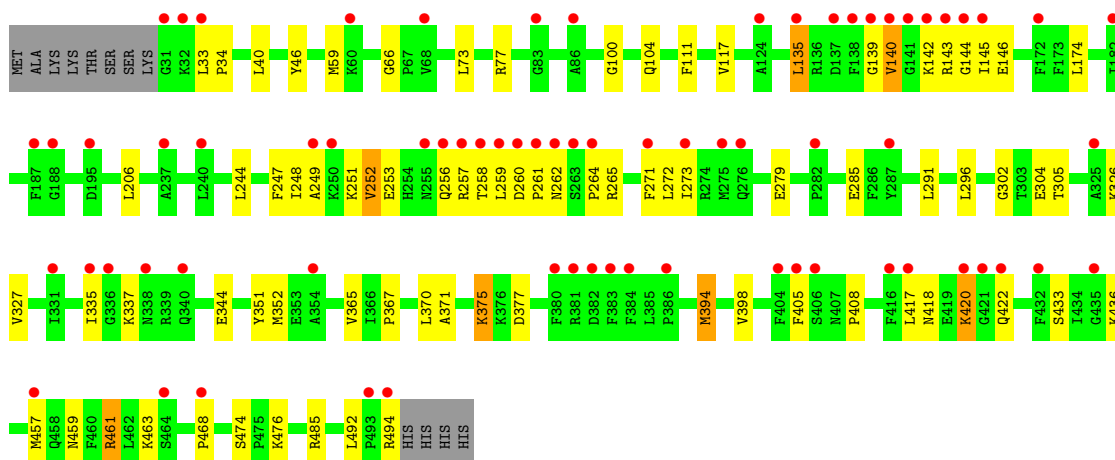
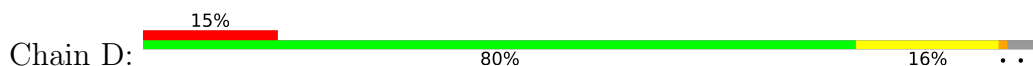
• Molecule 1: Cytochrome P450 2A6



● 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, α , β , γ	69.81Å 157.70Å 103.89Å 90.00° 92.23° 90.00°	Depositor
Resolution (Å)	50.00 – 1.85 50.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-1.85) 95.3 (50.00-1.85)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.73 (at 1.79Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.186 , 0.223 0.223 , 0.249	Depositor DCC
R_{free} test set	9625 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtrriage
Anisotropy	0.251	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16510	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: D1G, SO4, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.03	1/3851 (0.0%)	1.15	30/5186 (0.6%)
1	B	0.94	3/3838 (0.1%)	1.15	25/5170 (0.5%)
1	C	1.03	3/3842 (0.1%)	1.16	18/5175 (0.3%)
1	D	1.15	3/3842 (0.1%)	1.13	21/5175 (0.4%)
All	All	1.04	10/15373 (0.1%)	1.15	94/20706 (0.5%)

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	D	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	394	MET	SD-CE	-33.06	0.96	1.79
1	D	59	MET	SD-CE	-17.86	1.34	1.79
1	B	222	MET	SD-CE	-9.89	1.54	1.79
1	C	34	PRO	CA-C	9.53	1.57	1.51
1	C	205	MET	SD-CE	-8.31	1.58	1.79
1	D	34	PRO	CA-C	7.08	1.55	1.51
1	B	59	MET	SD-CE	-6.35	1.63	1.79
1	B	352	MET	SD-CE	-6.32	1.63	1.79
1	A	354	ALA	CA-CB	5.56	1.62	1.53
1	C	318	MET	SD-CE	5.35	1.93	1.79

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	304	GLU	N-CA-C	10.95	123.22	111.28
1	C	419	GLU	N-CA-C	-9.98	100.24	111.82
1	C	304	GLU	N-CA-C	9.90	122.15	111.36
1	D	304	GLU	N-CA-C	9.68	121.91	111.36
1	B	398	VAL	N-CA-C	-8.28	104.69	111.81
1	C	398	VAL	N-CA-C	-7.83	104.17	111.45
1	C	461	ARG	N-CA-C	-7.82	97.52	109.95
1	A	365	VAL	N-CA-C	7.59	118.36	110.62
1	A	381	ARG	CA-C-N	-7.22	111.71	122.83
1	A	381	ARG	C-N-CA	-7.22	111.71	122.83
1	D	398	VAL	N-CA-C	-7.22	104.73	111.45
1	D	104	GLN	N-CA-C	-7.04	93.85	107.44
1	D	66	GLY	CA-C-N	6.92	126.55	119.56
1	D	66	GLY	C-N-CA	6.92	126.55	119.56
1	B	234	GLN	CA-CB-CG	6.88	127.86	114.10
1	C	260	ASP	CA-C-N	6.78	128.31	119.84
1	C	260	ASP	C-N-CA	6.78	128.31	119.84
1	A	461	ARG	N-CA-C	-6.74	99.24	109.95
1	A	367	PRO	N-CA-C	6.61	122.44	113.84
1	B	234	GLN	CB-CA-C	-6.59	99.48	110.68
1	A	84	HIS	N-CA-C	6.58	119.01	111.11
1	A	104	GLN	N-CA-C	-6.56	94.78	107.44
1	C	173	PHE	N-CA-C	-6.49	104.21	111.28
1	B	173	PHE	N-CA-C	-6.46	104.15	111.07
1	D	370	LEU	N-CA-C	-6.46	99.18	109.59
1	C	104	GLN	N-CA-C	-6.39	95.11	107.44
1	C	370	LEU	N-CA-C	-6.32	99.39	109.76
1	A	370	LEU	N-CA-C	-6.29	98.94	109.07
1	B	104	GLN	N-CA-C	-6.22	95.43	107.44
1	B	365	VAL	N-CA-C	6.12	118.70	111.05
1	A	232	GLY	CA-C-N	6.06	125.95	119.28
1	A	232	GLY	C-N-CA	6.06	125.95	119.28
1	C	367	PRO	N-CA-C	5.99	121.74	113.65
1	B	105	ALA	N-CA-C	5.96	117.78	111.28
1	B	367	PRO	N-CA-C	5.96	121.59	113.84
1	D	371	ALA	N-CA-C	5.96	118.64	110.24
1	C	285	GLU	N-CA-C	-5.89	106.13	113.38
1	A	467	SER	CA-C-N	5.87	127.18	119.84
1	A	467	SER	C-N-CA	5.87	127.18	119.84
1	C	474	SER	N-CA-C	-5.85	101.70	110.24
1	C	288	LEU	N-CA-C	5.78	118.04	111.11
1	B	285	GLU	N-CA-C	-5.75	106.31	113.38
1	A	105	ALA	N-CA-C	5.75	117.54	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	482	THR	N-CA-C	-5.71	99.21	108.52
1	A	111	PHE	N-CA-C	5.70	117.57	111.36
1	D	474	SER	N-CA-C	-5.68	101.95	110.24
1	B	459	ASN	N-CA-C	5.57	120.14	113.23
1	D	367	PRO	N-CA-C	5.56	121.16	113.65
1	A	285	GLU	N-CA-C	-5.53	106.21	113.17
1	D	377	ASP	N-CA-C	-5.50	101.91	110.10
1	A	458	GLN	N-CA-C	-5.42	105.45	111.36
1	B	436	LYS	N-CA-C	5.42	118.11	111.82
1	D	461	ARG	N-CA-C	-5.41	101.35	109.95
1	B	223	PHE	N-CA-C	5.41	119.44	112.41
1	D	73	LEU	N-CA-C	-5.40	97.83	107.98
1	A	219	LEU	N-CA-C	-5.38	105.50	111.36
1	B	198	PHE	N-CA-C	-5.38	105.32	111.07
1	B	279	GLU	N-CA-C	5.37	122.23	110.80
1	A	338	ASN	N-CA-C	5.36	120.05	112.93
1	C	227	MET	N-CA-C	5.35	117.87	111.71
1	D	365	VAL	N-CA-C	5.33	117.71	111.05
1	B	219	LEU	N-CA-C	-5.32	105.48	111.28
1	B	66	GLY	CA-C-N	5.32	124.98	119.56
1	B	66	GLY	C-N-CA	5.32	124.98	119.56
1	A	116	VAL	N-CA-C	5.29	119.81	112.35
1	A	185	ILE	CB-CA-C	-5.25	105.14	112.02
1	B	461	ARG	N-CA-C	-5.25	101.60	109.95
1	D	335	ILE	N-CA-C	5.25	116.33	111.81
1	A	459	ASN	N-CA-C	5.25	119.74	113.23
1	D	436	LYS	N-CA-C	5.23	118.92	112.54
1	A	259	LEU	N-CA-C	5.23	117.80	109.96
1	D	100	GLY	N-CA-C	-5.19	105.66	112.82
1	D	34	PRO	CA-C-N	5.18	125.16	120.03
1	D	34	PRO	C-N-CA	5.18	125.16	120.03
1	A	34	PRO	N-CA-C	-5.18	104.38	110.70
1	A	385	LEU	CA-C-N	-5.17	114.45	119.78
1	A	385	LEU	C-N-CA	-5.17	114.45	119.78
1	C	168	ILE	N-CA-C	5.17	116.35	108.80
1	A	281	ASN	CA-C-N	5.17	124.97	119.28
1	A	281	ASN	C-N-CA	5.17	124.97	119.28
1	B	78	VAL	N-CA-C	5.16	115.33	108.11
1	B	185	ILE	CB-CA-C	-5.12	105.31	112.02
1	B	231	PRO	N-CA-C	-5.12	103.07	111.21
1	A	54	MET	N-CA-C	5.10	116.53	111.07
1	A	91	LEU	N-CA-C	5.10	118.60	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	GLY	N-CA-C	-5.09	101.95	112.34
1	B	474	SER	N-CA-C	-5.09	103.06	110.08
1	D	111	PHE	N-CA-C	5.09	117.95	111.69
1	C	392	TYR	CB-CA-C	-5.08	105.14	110.33
1	D	459	ASN	N-CA-C	5.08	119.53	113.23
1	D	285	GLU	N-CA-C	-5.07	107.14	113.38
1	A	393	PRO	N-CA-C	-5.06	102.35	110.74
1	C	141	GLY	N-CA-C	-5.05	108.28	115.30
1	C	117	VAL	N-CA-C	5.04	115.71	110.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	46	TYR	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	3760	0	3747	53	0
1	B	3747	0	3731	88	0
1	C	3751	0	3734	46	0
1	D	3751	0	3734	64	0
2	A	10	0	0	0	0
3	A	43	0	30	5	0
3	B	43	0	30	2	0
3	C	43	0	30	4	0
3	D	43	0	30	5	0
4	A	15	0	14	3	0
4	B	15	0	14	3	0
4	C	15	0	14	3	0
4	D	15	0	14	4	0
5	A	346	0	0	8	0
5	B	228	0	0	10	0
5	C	368	0	0	5	0
5	D	317	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	16510	0	15122	253	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 8.

All (253) 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:D:394:MET:CG	1:D:394:MET:CE	2.21	1.18
1:B:208:ILE:HD11	1:B:240:LEU:HB2	1.13	1.12
1:D:394:MET:CE	1:D:394:MET:SD	0.96	1.06
1:D:253:GLU:HG3	1:D:257:ARG:HH21	1.21	1.01
1:D:142:LYS:HG3	1:D:144:GLY:H	1.26	1.01
1:C:32:LYS:HB3	1:C:384:PHE:HB3	1.41	1.00
1:D:394:MET:SD	1:D:394:MET:HE1	1.58	1.00
1:C:418:ASN:HD22	1:C:422:GLN:HB2	1.28	0.99
1:D:394:MET:SD	1:D:394:MET:HE3	1.58	0.99
1:D:394:MET:SD	1:D:394:MET:HE2	1.58	0.97
1:D:139:GLY:O	1:D:142:LYS:HG2	1.65	0.95
1:A:30:LYS:HG2	1:A:382:ASP:O	1.65	0.95
1:A:30:LYS:HD3	1:A:32:LYS:HB3	1.53	0.91
1:A:32:LYS:HD2	1:A:33:LEU:H	1.35	0.90
1:B:77:ARG:HH12	1:B:389:THR:HG23	1.37	0.86
1:A:30:LYS:HG3	1:A:31:GLY:N	1.88	0.86
1:D:344:GLU:HG3	5:D:794:HOH:O	1.75	0.84
1:C:32:LYS:HE2	1:C:384:PHE:HB2	1.59	0.83
1:B:77:ARG:HG2	1:B:77:ARG:HH11	1.42	0.83
1:A:342:LYS:HE2	1:A:344:GLU:OE1	1.79	0.82
1:C:375:LYS:HB2	1:C:376:LYS:HE2	1.60	0.82
1:C:257:ARG:HH11	1:C:257:ARG:HG2	1.44	0.82
1:A:97:GLU:HG2	1:A:376:LYS:HE3	1.60	0.81
1:D:142:LYS:HG3	1:D:144:GLY:N	1.96	0.80
1:A:94:GLN:HG3	5:A:2700:HOH:O	1.81	0.80
1:B:208:ILE:CD1	1:B:240:LEU:HB2	2.05	0.80
1:B:53:GLN:HA	1:B:53:GLN:NE2	1.96	0.79
1:B:61:ILE:HD12	1:B:65:TYR:CD2	2.19	0.77
1:A:419:GLU:HA	1:A:419:GLU:OE1	1.83	0.75
1:B:37:PRO:HD3	1:B:61:ILE:HD13	1.69	0.74
1:B:64:ARG:HG2	1:B:64:ARG:HH11	1.52	0.72
1:D:375:LYS:HE2	5:D:545:HOH:O	1.88	0.72
1:A:346:ARG:HD2	1:A:353:GLU:OE1	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:LYS:HD2	5:B:629:HOH:O	1.89	0.71
1:B:202:LEU:HD23	1:B:205:MET:HE3	1.72	0.70
1:B:477:HIS:HD2	5:B:585:HOH:O	1.74	0.70
1:B:254:HIS:HA	1:B:257:ARG:HD2	1.73	0.69
1:C:125:LYS:NZ	1:C:129:ARG:HH12	1.90	0.69
1:B:305:THR:HG21	4:B:501:D1G:C12	2.23	0.68
1:D:253:GLU:HG3	1:D:257:ARG:NH2	2.02	0.68
1:A:125:LYS:HD2	5:A:2556:HOH:O	1.93	0.67
1:B:305:THR:HG21	4:B:501:D1G:H123	1.76	0.67
1:C:199:LEU:HD21	1:C:203:ARG:NH2	2.10	0.66
1:B:59:MET:HE1	1:B:82:CYS:SG	2.36	0.66
1:D:463:LYS:HD3	1:D:492:LEU:HD11	1.77	0.66
1:B:253:GLU:O	1:B:256:GLN:HG2	1.96	0.65
1:D:305:THR:HG21	4:D:501:D1G:C12	2.27	0.65
1:B:202:LEU:HD23	1:B:205:MET:CE	2.27	0.65
1:B:305:THR:HG23	5:B:587:HOH:O	1.96	0.64
1:D:305:THR:HG23	5:D:713:HOH:O	1.97	0.64
1:C:257:ARG:HH11	1:C:257:ARG:CG	2.12	0.63
1:A:30:LYS:HG3	1:A:32:LYS:H	1.64	0.63
1:B:53:GLN:NE2	1:B:478:VAL:HB	2.14	0.62
1:B:208:ILE:HD11	1:B:240:LEU:CB	2.09	0.62
1:C:400:ARG:HD2	5:C:761:HOH:O	2.00	0.61
1:B:210:GLN:O	1:B:214:THR:HG23	1.99	0.61
1:C:414:GLN:HG3	5:C:863:HOH:O	2.00	0.61
1:C:418:ASN:HB2	1:C:422:GLN:H	1.66	0.61
1:B:33:LEU:HD12	1:B:34:PRO:HD2	1.82	0.60
1:B:77:ARG:HH11	1:B:77:ARG:CG	2.07	0.60
1:B:61:ILE:HD11	1:B:69:PHE:CD1	2.37	0.60
1:A:60:LYS:HE2	5:A:2796:HOH:O	2.02	0.60
1:D:420:LYS:HG3	1:D:422:GLN:OE1	2.02	0.60
1:D:253:GLU:CG	1:D:257:ARG:HH21	2.07	0.60
1:C:322:GLU:O	1:C:326:LYS:HG3	2.02	0.59
1:A:302:GLY:HA2	3:A:500:HEM:HMC3	1.84	0.59
1:A:112:LYS:NZ	5:A:2809:HOH:O	2.36	0.58
1:B:450:PHE:O	1:B:454:THR:HG23	2.03	0.58
1:D:394:MET:HE2	1:D:394:MET:HA	1.85	0.58
1:C:375:LYS:CB	1:C:376:LYS:HE2	2.31	0.58
1:B:233:PRO:O	1:B:236:GLN:HG3	2.03	0.58
1:A:30:LYS:HG3	1:A:31:GLY:H	1.66	0.58
1:B:254:HIS:O	1:B:258:THR:HG22	2.03	0.58
1:B:327:VAL:HG13	1:B:352:MET:HE1	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ARG:HD2	1:A:353:GLU:CD	2.29	0.57
1:B:61:ILE:HD12	1:B:65:TYR:HD2	1.69	0.57
1:D:143:ARG:HA	1:D:146:GLU:HB3	1.86	0.57
1:D:140:VAL:HA	1:D:145:ILE:HG21	1.86	0.57
1:D:327:VAL:HG11	1:D:457:MET:CE	2.34	0.57
1:B:172:PHE:O	1:B:176:ARG:HG3	2.05	0.56
1:D:271:PHE:HB3	1:D:291:LEU:HD13	1.86	0.56
1:A:30:LYS:CD	1:A:32:LYS:HB3	2.33	0.56
1:C:305:THR:HG21	4:C:501:D1G:C12	2.36	0.56
1:A:206:LEU:HD12	5:A:2779:HOH:O	2.04	0.56
1:B:49:LEU:HD12	1:B:222:MET:HE1	1.86	0.56
1:C:32:LYS:HB3	1:C:384:PHE:CB	2.27	0.56
1:A:40:LEU:HD11	1:C:47:LEU:HD11	1.88	0.56
1:A:305:THR:HG21	4:A:501:D1G:C12	2.36	0.55
1:D:271:PHE:CG	1:D:291:LEU:HD13	2.41	0.55
1:B:200:SER:O	1:B:204:MET:HG3	2.05	0.55
1:A:342:LYS:CE	1:A:344:GLU:OE1	2.53	0.55
1:D:461:ARG:HG3	1:D:492:LEU:HB2	1.87	0.55
1:B:461:ARG:NH1	1:B:493:PRO:O	2.40	0.54
1:A:465:SER:HB2	5:B:670:HOH:O	2.05	0.54
1:C:346:ARG:HG2	1:C:353:GLU:OE1	2.08	0.54
1:D:461:ARG:HH12	1:D:494:ARG:HA	1.73	0.54
1:A:32:LYS:CD	1:A:33:LEU:H	2.15	0.54
1:B:259:LEU:HD12	1:B:260:ASP:H	1.72	0.53
1:B:64:ARG:HG2	1:B:64:ARG:NH1	2.22	0.53
1:D:327:VAL:HG13	1:D:352:MET:HE2	1.90	0.53
1:A:305:THR:HG23	5:A:2568:HOH:O	2.09	0.53
3:C:500:HEM:NC	4:C:501:D1G:H111	2.24	0.53
1:C:76:ARG:NH2	1:C:103:GLU:HG3	2.24	0.52
1:B:143:ARG:O	1:B:147:GLU:HG3	2.09	0.52
1:B:53:GLN:HE22	1:B:478:VAL:HB	1.75	0.52
1:C:302:GLY:HA2	3:C:500:HEM:HMC3	1.91	0.52
1:A:357:HIS:NE2	1:A:446:ARG:NH2	2.56	0.52
1:C:33:LEU:HD11	1:C:77:ARG:CZ	2.40	0.52
1:D:461:ARG:NH1	1:D:494:ARG:HA	2.25	0.52
1:D:206:LEU:HD12	5:D:611:HOH:O	2.08	0.52
1:D:476:LYS:HB2	1:D:485:ARG:HA	1.91	0.52
1:B:73:LEU:HA	1:B:222:MET:CE	2.40	0.51
1:B:469:LYS:HG3	1:B:470:ASP:N	2.24	0.51
1:D:142:LYS:CG	1:D:144:GLY:H	2.10	0.51
1:C:305:THR:HG23	5:C:574:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:HD11	1:A:77:ARG:CZ	2.41	0.51
1:B:37:PRO:CD	1:B:61:ILE:HD13	2.41	0.51
1:D:139:GLY:O	1:D:142:LYS:CG	2.50	0.51
1:D:260:ASP:O	1:D:262:ASN:N	2.44	0.51
1:C:369:SER:HB2	1:C:395:LEU:HG	1.92	0.51
1:B:352:MET:HE3	1:B:454:THR:HG22	1.93	0.50
1:B:337:LYS:HG2	5:B:626:HOH:O	2.10	0.50
1:D:244:LEU:HB3	1:D:296:LEU:HD11	1.93	0.50
1:B:327:VAL:HG11	1:B:457:MET:CE	2.42	0.50
1:B:57:SER:O	1:B:61:ILE:HG23	2.12	0.50
1:D:248:ILE:O	1:D:252:VAL:HG12	2.12	0.49
1:D:252:VAL:O	1:D:256:GLN:HG3	2.13	0.49
1:A:208:ILE:HD13	1:A:241:LEU:CD2	2.43	0.49
1:A:208:ILE:HD13	1:A:241:LEU:HD23	1.95	0.49
1:D:271:PHE:CB	1:D:291:LEU:HD13	2.43	0.49
1:A:305:THR:HG21	4:A:501:D1G:H123	1.95	0.49
1:B:73:LEU:HA	1:B:222:MET:HE2	1.95	0.49
1:B:76:ARG:CZ	1:B:103:GLU:HG3	2.43	0.48
1:C:76:ARG:CZ	1:C:103:GLU:HG3	2.43	0.48
1:D:394:MET:HE2	1:D:394:MET:CA	2.43	0.48
1:A:376:LYS:HD3	1:A:376:LYS:N	2.29	0.48
1:C:418:ASN:CB	1:C:422:GLN:H	2.27	0.48
1:A:433:SER:HB3	3:A:500:HEM:HBA1	1.95	0.48
1:B:77:ARG:CG	1:B:77:ARG:NH1	2.68	0.48
1:B:354:ALA:HB2	1:B:417:LEU:HD13	1.95	0.48
1:B:59:MET:O	1:B:62:SER:OG	2.29	0.47
1:C:168:ILE:C	1:C:168:ILE:HD12	2.39	0.47
1:D:247:PHE:O	1:D:251:LYS:HG2	2.14	0.47
1:D:253:GLU:O	1:D:256:GLN:HB2	2.15	0.47
1:B:274:ARG:NH2	5:B:695:HOH:O	2.47	0.47
1:A:55:TYR:CZ	1:A:400:ARG:NH2	2.83	0.47
1:A:194:LYS:NZ	5:A:2837:HOH:O	2.47	0.47
1:D:405:PHE:O	1:D:408:PRO:HD3	2.14	0.47
1:D:139:GLY:C	1:D:142:LYS:HG2	2.37	0.47
1:B:77:ARG:HH12	1:B:389:THR:CG2	2.18	0.47
1:C:418:ASN:HB2	1:C:422:GLN:N	2.30	0.47
1:B:327:VAL:HG13	1:B:352:MET:CE	2.45	0.47
1:B:405:PHE:O	1:B:408:PRO:HD3	2.15	0.47
1:D:117:VAL:HG22	3:D:500:HEM:HAD1	1.96	0.47
1:D:305:THR:HG21	4:D:501:D1G:H123	1.96	0.46
1:D:326:LYS:HE2	1:D:351:TYR:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:SER:HB3	3:B:500:HEM:HBA1	1.96	0.46
1:A:95:ALA:HB1	1:A:436:LYS:HG3	1.98	0.46
1:A:291:LEU:HD12	1:A:291:LEU:O	2.16	0.46
1:C:125:LYS:NZ	1:C:129:ARG:NH1	2.63	0.46
1:D:135:LEU:HD12	1:D:135:LEU:HA	1.77	0.46
1:D:326:LYS:HE3	5:D:817:HOH:O	2.15	0.46
1:B:74:GLY:H	1:B:222:MET:HE2	1.80	0.46
1:B:77:ARG:NH1	1:B:389:THR:HG23	2.17	0.46
1:D:327:VAL:HG11	1:D:457:MET:SD	2.55	0.46
1:B:77:ARG:NE	5:B:678:HOH:O	2.48	0.45
1:A:384:PHE:C	1:A:385:LEU:HD12	2.42	0.45
1:D:305:THR:HG21	4:D:501:D1G:H122	1.98	0.45
1:A:357:HIS:CE1	1:A:446:ARG:NH2	2.84	0.45
1:C:76:ARG:HG2	1:C:390:GLU:OE1	2.16	0.45
1:C:117:VAL:HG22	3:C:500:HEM:HAD1	1.97	0.45
1:C:327:VAL:HG13	1:C:352:MET:HE2	1.97	0.45
1:A:342:LYS:HE2	1:A:344:GLU:CG	2.46	0.45
1:B:377:ASP:HB3	1:B:384:PHE:CE1	2.52	0.45
1:C:257:ARG:CG	1:C:257:ARG:NH1	2.74	0.45
1:D:433:SER:HB3	3:D:500:HEM:HBA1	1.98	0.45
1:D:249:ALA:HA	1:D:252:VAL:CG1	2.47	0.45
1:A:123:ARG:HA	1:A:285:GLU:HG3	1.98	0.45
1:B:74:GLY:N	1:B:222:MET:HE2	2.31	0.45
1:D:326:LYS:HE2	1:D:351:TYR:CE1	2.52	0.45
1:A:89:GLU:O	1:A:93:ASP:HB2	2.17	0.45
1:B:143:ARG:HD2	1:B:146:GLU:OE2	2.17	0.45
1:B:148:ARG:HA	1:B:148:ARG:HD3	1.76	0.45
1:A:441:GLY:HA3	3:A:500:HEM:C3C	2.53	0.44
1:B:258:THR:HG23	1:B:265:ARG:HH22	1.82	0.44
1:B:260:ASP:HB2	1:B:263:SER:HB3	1.98	0.44
3:D:500:HEM:C1D	4:D:501:D1G:H113	2.52	0.44
1:A:274:ARG:HA	1:A:274:ARG:HD2	1.73	0.44
1:A:342:LYS:HE2	1:A:344:GLU:CD	2.42	0.44
1:A:97:GLU:CG	1:A:376:LYS:HE3	2.40	0.44
1:B:37:PRO:HD3	1:B:61:ILE:CD1	2.43	0.44
1:B:196:LYS:HD2	5:B:703:HOH:O	2.16	0.44
1:C:346:ARG:CG	1:C:353:GLU:OE1	2.65	0.44
1:D:418:ASN:OD1	1:D:420:LYS:HG2	2.18	0.44
1:C:125:LYS:HZ3	1:C:129:ARG:NH1	2.16	0.44
1:C:355:VAL:O	1:C:359:ILE:HG13	2.17	0.44
1:A:94:GLN:NE2	5:A:2700:HOH:O	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:SER:O	1:B:468:PRO:C	2.60	0.43
1:B:469:LYS:HE3	1:B:470:ASP:OD1	2.18	0.43
1:C:210:GLN:HB3	5:C:779:HOH:O	2.18	0.43
1:D:258:THR:OG1	1:D:265:ARG:NH1	2.45	0.43
1:A:239:GLN:HA	1:A:239:GLN:OE1	2.18	0.43
1:B:140:VAL:HA	1:B:145:ILE:HG21	2.00	0.43
1:C:103:GLU:HB2	1:C:108:ASP:OD2	2.18	0.43
1:D:264:PRO:HG3	1:D:273:ILE:CD1	2.49	0.43
1:B:139:GLY:C	1:B:145:ILE:HB	2.43	0.43
1:C:305:THR:HG21	4:C:501:D1G:H123	2.00	0.43
1:C:476:LYS:HB2	1:C:485:ARG:HA	2.01	0.43
1:A:291:LEU:HD12	1:A:291:LEU:C	2.44	0.43
1:B:375:LYS:HB3	1:B:375:LYS:HE3	1.85	0.43
1:B:446:ARG:HH11	1:B:446:ARG:HB3	1.84	0.43
1:D:394:MET:CG	1:D:394:MET:HE2	2.21	0.43
1:A:117:VAL:HG22	3:A:500:HEM:HAD1	2.01	0.43
1:A:200:SER:O	1:A:204:MET:HG3	2.19	0.42
1:A:463:LYS:HB3	1:A:490:SER:OG	2.18	0.42
1:B:204:MET:O	1:B:208:ILE:HG12	2.18	0.42
1:B:297:ASN:HA	4:B:501:D1G:N_1	2.35	0.42
1:C:375:LYS:HB2	1:C:376:LYS:CE	2.41	0.42
1:D:302:GLY:HA2	3:D:500:HEM:HMC3	2.00	0.42
3:D:500:HEM:HBB2	3:D:500:HEM:HMB2	2.00	0.42
1:D:272:LEU:HD23	1:D:272:LEU:HA	1.89	0.42
1:B:319:LYS:C	1:B:321:PRO:HD3	2.45	0.42
1:A:186:VAL:HA	1:A:267:PHE:HB3	2.02	0.41
1:B:253:GLU:HA	1:B:256:GLN:HG2	2.01	0.41
1:B:363:GLY:O	1:B:364:ASP:C	2.62	0.41
1:C:136:ARG:HG2	5:C:841:HOH:O	2.20	0.41
1:C:376:LYS:HE3	1:C:376:LYS:HB2	1.78	0.41
1:C:441:GLY:HA3	3:C:500:HEM:C3C	2.55	0.41
1:B:254:HIS:O	1:B:257:ARG:HG2	2.21	0.41
1:D:142:LYS:HE2	1:D:144:GLY:H	1.84	0.41
1:D:249:ALA:HA	1:D:252:VAL:HG12	2.03	0.41
1:A:30:LYS:CG	1:A:32:LYS:H	2.31	0.41
1:B:77:ARG:CD	5:B:678:HOH:O	2.68	0.41
1:B:258:THR:HG23	1:B:265:ARG:HH12	1.84	0.41
1:B:97:GLU:OE1	1:B:378:THR:HG23	2.21	0.41
1:B:436:LYS:HE3	1:B:436:LYS:HB3	1.78	0.41
1:B:467:SER:O	1:B:470:ASP:N	2.53	0.41
3:A:500:HEM:C1D	4:A:501:D1G:H113	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:GLN:HG2	5:B:666:HOH:O	2.21	0.41
1:B:377:ASP:HB3	1:B:384:PHE:CZ	2.56	0.41
1:C:418:ASN:ND2	1:C:422:GLN:HB2	2.12	0.40
1:A:52:GLU:OE1	1:B:236:GLN:HG2	2.21	0.40
1:B:302:GLY:HA2	3:B:500:HEM:HMC3	2.03	0.40
1:D:259:LEU:HD12	1:D:260:ASP:N	2.36	0.40
1:D:394:MET:CE	1:D:394:MET:HG2	2.38	0.40
1:B:145:ILE:HD12	1:B:145:ILE:HA	1.72	0.40
1:C:145:ILE:HD12	1:C:145:ILE:HA	1.86	0.40
1:C:152:GLU:HG3	1:C:177:THR:HG23	2.03	0.40
1:C:345:ASP:O	1:C:349:MET:HG3	2.20	0.40
1:D:33:LEU:HD11	1:D:77:ARG:CZ	2.52	0.40
1:B:369:SER:HB2	1:B:395:LEU:HG	2.02	0.40
1:D:264:PRO:HG3	1:D:273:ILE:HD12	2.04	0.40
1:D:420:LYS:HG2	1:D:420:LYS:H	1.58	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%)	452 (98%)	11 (2%)	0	100	100
1	B	461/476 (97%)	446 (97%)	14 (3%)	1 (0%)	43	31
1	C	462/476 (97%)	451 (98%)	11 (2%)	0	100	100
1	D	462/476 (97%)	442 (96%)	18 (4%)	2 (0%)	30	17
All	All	1848/1904 (97%)	1791 (97%)	54 (3%)	3 (0%)	43	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	140	VAL
1	B	261	PRO
1	D	261	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	412/422 (98%)	402 (98%)	10 (2%)	43	28
1	B	411/422 (97%)	394 (96%)	17 (4%)	27	12
1	C	411/422 (97%)	406 (99%)	5 (1%)	63	55
1	D	411/422 (97%)	401 (98%)	10 (2%)	43	28
All	All	1645/1688 (98%)	1603 (97%)	42 (3%)	40	25

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	135	LEU
1	A	167	ASN
1	A	189	ASP
1	A	236	GLN
1	A	291	LEU
1	A	348	LYS
1	A	376	LYS
1	A	419	GLU
1	A	468	PRO
1	B	33	LEU
1	B	52	GLU
1	B	53	GLN
1	B	61	ILE
1	B	135	LEU
1	B	145	ILE
1	B	174	LEU
1	B	210	GLN
1	B	234	GLN

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Mol	Chain	Res	Type
1	B	260	ASP
1	B	261	PRO
1	B	316	LEU
1	B	417	LEU
1	B	419	GLU
1	B	446	ARG
1	B	467	SER
1	B	468	PRO
1	C	135	LEU
1	C	148	ARG
1	C	210	GLN
1	C	376	LYS
1	C	417	LEU
1	D	40	LEU
1	D	135	LEU
1	D	174	LEU
1	D	252	VAL
1	D	279	GLU
1	D	337	LYS
1	D	375	LYS
1	D	417	LEU
1	D	420	LYS
1	D	468	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	276	GLN
1	A	283	ASN
1	A	297	ASN
1	A	407	ASN
1	B	72	HIS
1	B	255	ASN
1	B	297	ASN
1	B	320	HIS
1	B	338	ASN
1	B	414	GLN
1	C	297	ASN
1	C	320	HIS
1	C	328	HIS
1	C	409	GLN

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Mol	Chain	Res	Type
1	C	418	ASN
1	C	422	GLN
1	D	53	GLN
1	D	56	ASN
1	D	236	GLN
1	D	297	ASN
1	D	338	ASN
1	D	340	GLN
1	D	409	GLN
1	D	466	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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
4	D1G	B	501	3	16,16,16	1.71	5 (31%)	21,21,21	1.22	1 (4%)
4	D1G	A	501	3	16,16,16	1.71	4 (25%)	21,21,21	0.90	1 (4%)
3	HEM	B	500	4,1	50,50,50	2.27	26 (52%)	67,82,82	1.16	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	D1G	C	501	3	16,16,16	1.48	2 (12%)	21,21,21	1.06	1 (4%)
4	D1G	D	501	3	16,16,16	1.53	3 (18%)	21,21,21	1.00	1 (4%)
2	SO4	A	2503	-	4,4,4	0.79	0	6,6,6	0.27	0
2	SO4	A	2502	-	4,4,4	0.73	0	6,6,6	0.42	0
3	HEM	A	500	4,1	50,50,50	2.39	22 (44%)	67,82,82	1.21	7 (10%)
3	HEM	D	500	4,1	50,50,50	2.32	24 (48%)	67,82,82	1.11	3 (4%)
3	HEM	C	500	4,1	50,50,50	2.18	22 (44%)	67,82,82	1.18	6 (8%)

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
4	D1G	B	501	3	-	0/8/8/8	0/2/2/2
4	D1G	A	501	3	-	0/8/8/8	0/2/2/2
3	HEM	B	500	4,1	-	4/14/54/54	-
4	D1G	C	501	3	-	0/8/8/8	0/2/2/2
4	D1G	D	501	3	-	0/8/8/8	0/2/2/2
3	HEM	A	500	4,1	-	3/14/54/54	-
3	HEM	D	500	4,1	-	4/14/54/54	-
3	HEM	C	500	4,1	-	5/14/54/54	-

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	HEM	C1D-ND	-5.05	1.28	1.38
3	A	500	HEM	C4D-ND	-4.59	1.32	1.40
3	D	500	HEM	C4A-NA	-4.56	1.31	1.39
3	C	500	HEM	CMA-C3A	4.54	1.60	1.50
3	A	500	HEM	FE-ND	4.52	2.08	1.94
3	A	500	HEM	C4A-NA	-4.47	1.31	1.39
3	B	500	HEM	C4D-ND	-4.14	1.33	1.40
3	D	500	HEM	C1B-NB	-4.03	1.33	1.40
3	D	500	HEM	FE-NA	4.02	2.08	1.95
3	A	500	HEM	CMD-C2D	3.99	1.58	1.50
3	C	500	HEM	FE-NB	3.84	2.06	1.94
3	C	500	HEM	FE-ND	3.81	2.06	1.94
3	B	500	HEM	FE-NA	3.79	2.07	1.95
3	D	500	HEM	FE-NB	3.77	2.06	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	HEM	CMA-C3A	3.76	1.58	1.50
3	D	500	HEM	C1C-C2C	-3.74	1.37	1.45
3	B	500	HEM	C1D-ND	-3.73	1.31	1.38
3	A	500	HEM	CAC-C3C	-3.64	1.37	1.47
3	C	500	HEM	C4D-ND	-3.63	1.34	1.40
3	A	500	HEM	C4D-C3D	-3.58	1.39	1.45
3	D	500	HEM	CMD-C2D	3.56	1.58	1.50
3	B	500	HEM	CMB-C2B	3.55	1.58	1.50
3	D	500	HEM	CMA-C3A	3.54	1.58	1.50
3	C	500	HEM	C1D-ND	-3.50	1.32	1.38
4	A	501	D1G	C_2-C_1	3.49	1.44	1.39
3	B	500	HEM	CMA-C3A	3.41	1.57	1.50
3	A	500	HEM	CMC-C2C	3.40	1.57	1.50
3	B	500	HEM	C4A-NA	-3.38	1.33	1.39
3	A	500	HEM	FE-NB	3.37	2.05	1.94
3	D	500	HEM	CAC-C3C	-3.36	1.38	1.47
3	B	500	HEM	FE-ND	3.34	2.05	1.94
3	A	500	HEM	C1C-NC	-3.33	1.33	1.39
3	D	500	HEM	C3C-C4C	-3.31	1.40	1.46
3	A	500	HEM	CBB-CAB	3.28	1.46	1.30
3	C	500	HEM	CAC-C3C	-3.26	1.38	1.47
3	A	500	HEM	C1B-NB	-3.26	1.34	1.40
3	B	500	HEM	C1D-C2D	-3.26	1.37	1.44
3	B	500	HEM	CMC-C2C	3.20	1.57	1.50
3	C	500	HEM	FE-NC	3.16	2.05	1.95
3	D	500	HEM	C1C-NC	-3.14	1.33	1.39
3	D	500	HEM	FE-NC	3.14	2.05	1.95
3	B	500	HEM	CAC-C3C	-3.14	1.39	1.47
3	C	500	HEM	C1D-C2D	-3.13	1.38	1.44
3	D	500	HEM	C1A-C2A	-3.11	1.38	1.44
3	B	500	HEM	C1C-C2C	-3.10	1.39	1.45
3	B	500	HEM	C3B-C2B	3.09	1.43	1.37
4	C	501	D1G	C_1-C_6	-3.07	1.41	1.48
3	C	500	HEM	C4D-C3D	-3.06	1.39	1.45
3	B	500	HEM	FE-NB	3.06	2.04	1.94
4	A	501	D1G	C_1-C_6	-3.06	1.41	1.48
4	B	501	D1G	C_2-C_1	3.05	1.44	1.39
3	D	500	HEM	C3B-C4B	-3.03	1.39	1.44
3	B	500	HEM	CBB-CAB	3.03	1.44	1.30
3	A	500	HEM	FE-NA	3.02	2.05	1.95
3	D	500	HEM	FE-ND	3.02	2.04	1.94
3	C	500	HEM	C3B-C2B	3.01	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	HEM	C1C-C2C	-3.01	1.39	1.45
3	D	500	HEM	CMC-C2C	2.99	1.56	1.50
3	B	500	HEM	C1C-NC	-2.98	1.34	1.39
3	A	500	HEM	CBD-CGD	2.98	1.57	1.50
3	D	500	HEM	CBB-CAB	2.96	1.44	1.30
3	D	500	HEM	O2A-CGA	-2.96	1.21	1.30
4	B	501	D1G	C_5-C_1	2.93	1.43	1.39
3	B	500	HEM	C4D-C3D	-2.92	1.40	1.45
4	D	501	D1G	C_1-C_6	-2.89	1.41	1.48
3	C	500	HEM	FE-NA	2.88	2.04	1.95
3	A	500	HEM	C1A-C2A	-2.86	1.38	1.44
3	B	500	HEM	C3C-C4C	-2.84	1.41	1.46
4	D	501	D1G	C_5-C_1	2.82	1.43	1.39
3	C	500	HEM	CBB-CAB	2.76	1.43	1.30
3	C	500	HEM	C1A-C2A	-2.76	1.39	1.44
4	C	501	D1G	C_2-C_1	2.74	1.43	1.39
3	C	500	HEM	C4A-NA	-2.71	1.34	1.39
3	C	500	HEM	C1C-C2C	-2.71	1.40	1.45
3	D	500	HEM	C4D-ND	-2.68	1.35	1.40
4	B	501	D1G	C_1-C_6	-2.61	1.42	1.48
3	C	500	HEM	C3B-C4B	-2.56	1.40	1.44
4	B	501	D1G	C_7-C_6	2.51	1.40	1.35
3	A	500	HEM	C3C-C4C	-2.48	1.41	1.46
3	A	500	HEM	FE-NC	2.46	2.03	1.95
3	D	500	HEM	C4D-C3D	-2.45	1.40	1.45
4	D	501	D1G	C_2-C_1	2.44	1.43	1.39
3	C	500	HEM	CMC-C2C	2.39	1.55	1.50
4	A	501	D1G	C_3-C_4	2.35	1.44	1.37
3	C	500	HEM	CHD-C4C	2.35	1.43	1.38
3	A	500	HEM	C1D-C2D	-2.35	1.39	1.44
3	D	500	HEM	C3C-C2C	2.34	1.41	1.37
3	C	500	HEM	CBC-CAC	2.33	1.41	1.30
3	B	500	HEM	FE-NC	2.30	2.02	1.95
3	D	500	HEM	C4C-NC	-2.29	1.35	1.39
3	A	500	HEM	C4B-NB	-2.27	1.34	1.38
3	B	500	HEM	C4B-NB	-2.24	1.34	1.38
3	D	500	HEM	C3B-C2B	2.21	1.41	1.37
3	D	500	HEM	C1D-ND	-2.20	1.34	1.38
3	C	500	HEM	C1C-NC	-2.15	1.35	1.39
3	B	500	HEM	C4C-NC	-2.15	1.35	1.39
3	B	500	HEM	CBC-CAC	2.14	1.40	1.30
4	A	501	D1G	C_5-C_1	2.13	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	D1G	O_1-C_6	2.11	1.42	1.38
3	B	500	HEM	C1A-NA	-2.11	1.35	1.39
3	B	500	HEM	CBD-CGD	2.10	1.55	1.50
3	A	500	HEM	C4C-NC	-2.08	1.35	1.39
3	B	500	HEM	CMD-C2D	2.07	1.55	1.50
3	C	500	HEM	C4B-NB	-2.07	1.34	1.38
3	C	500	HEM	C3C-C4C	-2.07	1.42	1.46
3	B	500	HEM	CHD-C1D	-2.06	1.34	1.39
3	B	500	HEM	O2A-CGA	-2.03	1.24	1.30
3	D	500	HEM	CHD-C1D	-2.03	1.34	1.39

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	D1G	C_6-O_1-C_9	-4.36	104.61	106.93
3	C	500	HEM	CHD-C4C-NC	-3.48	120.67	124.45
4	C	501	D1G	C_6-O_1-C_9	-3.25	105.19	106.93
3	B	500	HEM	C3B-C4B-NB	3.12	111.71	109.47
3	A	500	HEM	O2A-CGA-CBA	3.06	123.65	114.00
3	C	500	HEM	O2A-CGA-CBA	3.00	123.47	114.00
3	B	500	HEM	C3B-C2B-C1B	-2.93	104.21	106.41
4	D	501	D1G	C_6-O_1-C_9	-2.83	105.42	106.93
3	A	500	HEM	CHB-C1B-NB	-2.81	120.89	124.37
3	D	500	HEM	C3B-C4B-NB	2.70	111.41	109.47
3	A	500	HEM	C3B-C4B-NB	2.66	111.38	109.47
3	D	500	HEM	O2A-CGA-CBA	2.64	122.33	114.00
3	D	500	HEM	CHD-C4C-NC	-2.59	121.63	124.45
3	A	500	HEM	C4B-C3B-C2B	-2.58	104.91	107.28
3	C	500	HEM	C3B-C2B-C1B	-2.57	104.48	106.41
3	B	500	HEM	CHD-C4C-NC	-2.53	121.70	124.45
3	B	500	HEM	O2A-CGA-CBA	2.46	121.76	114.00
3	C	500	HEM	C3B-C4B-NB	2.45	111.23	109.47
3	C	500	HEM	C1C-CHC-C4B	2.35	131.00	126.02
3	A	500	HEM	O1A-CGA-CBA	-2.32	115.73	123.09
3	A	500	HEM	C4D-ND-C1D	2.28	107.91	105.21
3	B	500	HEM	C4D-ND-C1D	2.21	107.83	105.21
3	C	500	HEM	O1A-CGA-CBA	-2.09	116.47	123.09
3	A	500	HEM	C4A-CHB-C1B	2.05	131.07	126.25
4	A	501	D1G	C_6-O_1-C_9	-2.05	105.84	106.93
3	B	500	HEM	CHB-C1B-NB	-2.03	121.86	124.37

There are no chirality outliers.

All (16) torsion outliers are listed below:

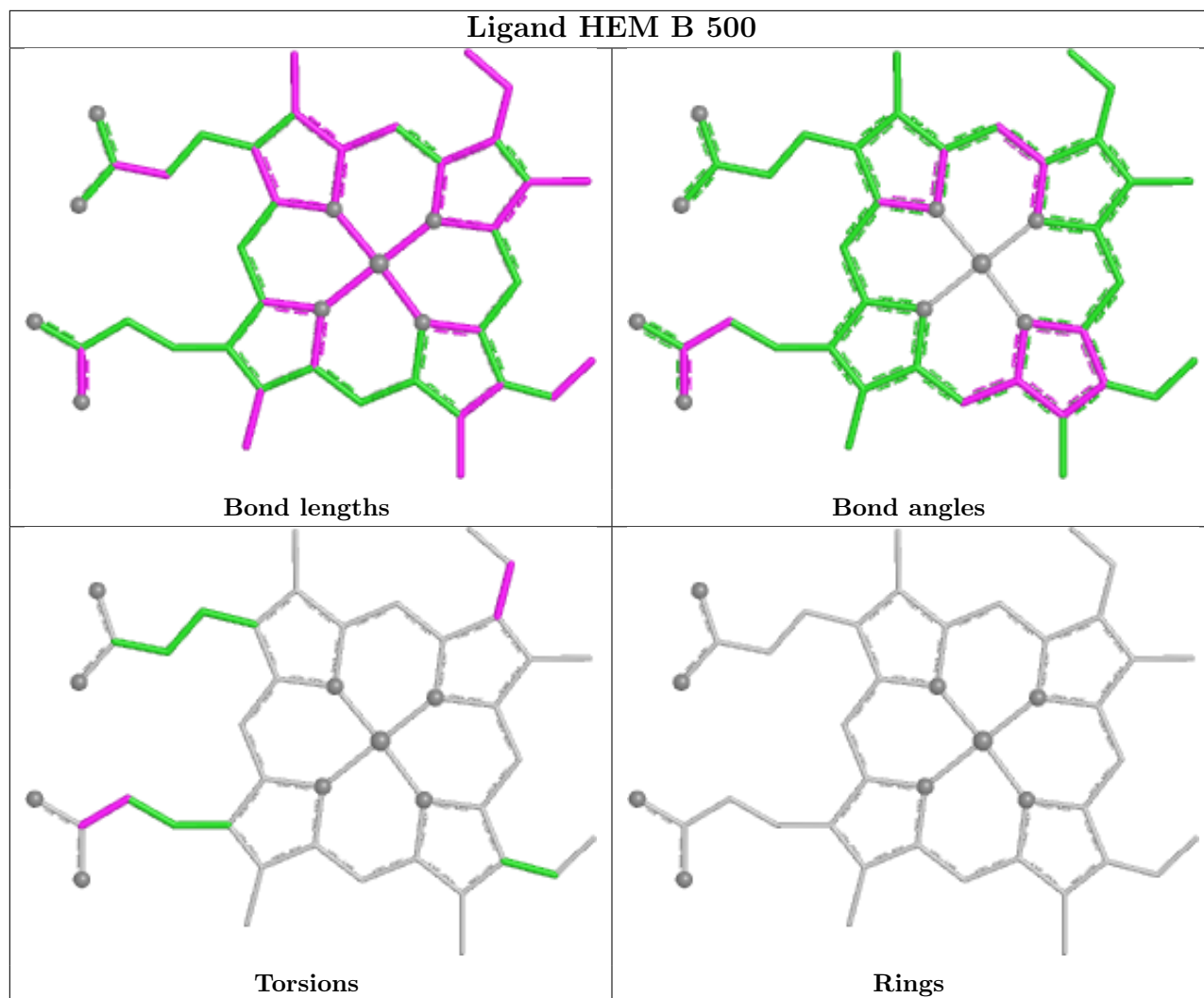
Mol	Chain	Res	Type	Atoms
3	B	500	HEM	C2C-C3C-CAC-CBC
3	B	500	HEM	C4C-C3C-CAC-CBC
3	A	500	HEM	C2C-C3C-CAC-CBC
3	C	500	HEM	C2C-C3C-CAC-CBC
3	A	500	HEM	C4C-C3C-CAC-CBC
3	B	500	HEM	CAA-CBA-CGA-O1A
3	C	500	HEM	C4C-C3C-CAC-CBC
3	D	500	HEM	C4C-C3C-CAC-CBC
3	D	500	HEM	CAA-CBA-CGA-O1A
3	D	500	HEM	CAA-CBA-CGA-O2A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

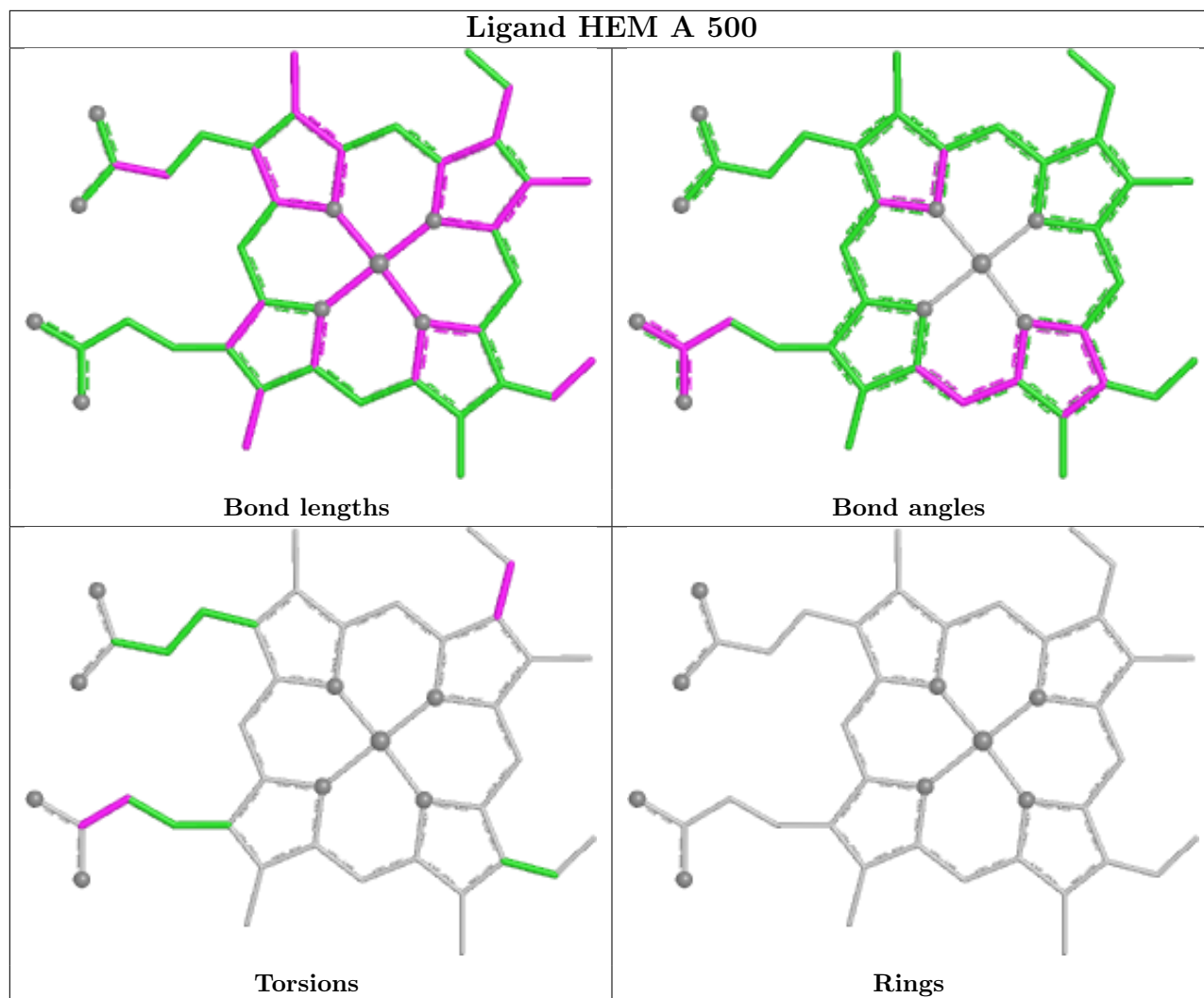
There are no ring outliers.

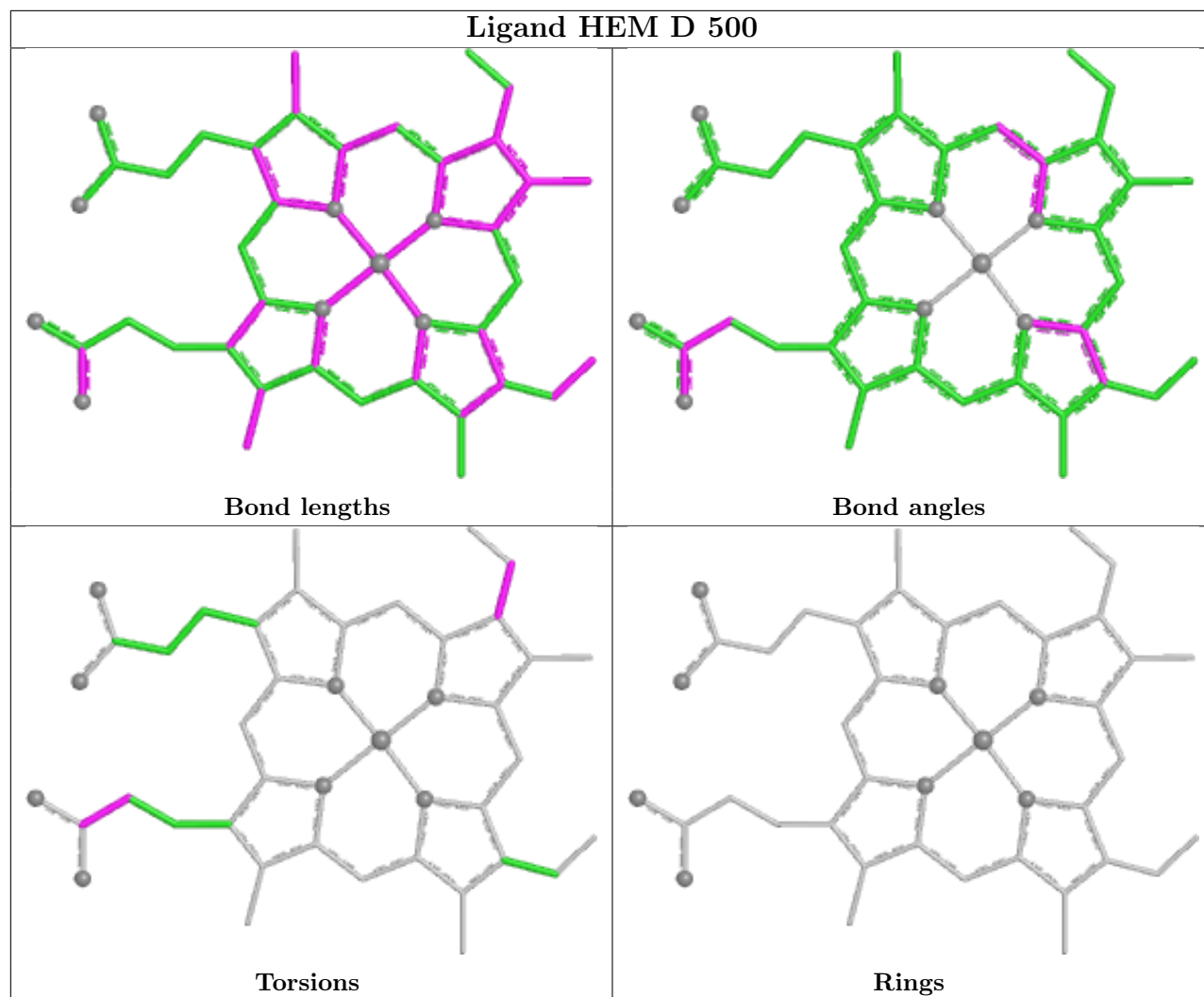
8 monomers are involved in 26 short contacts:

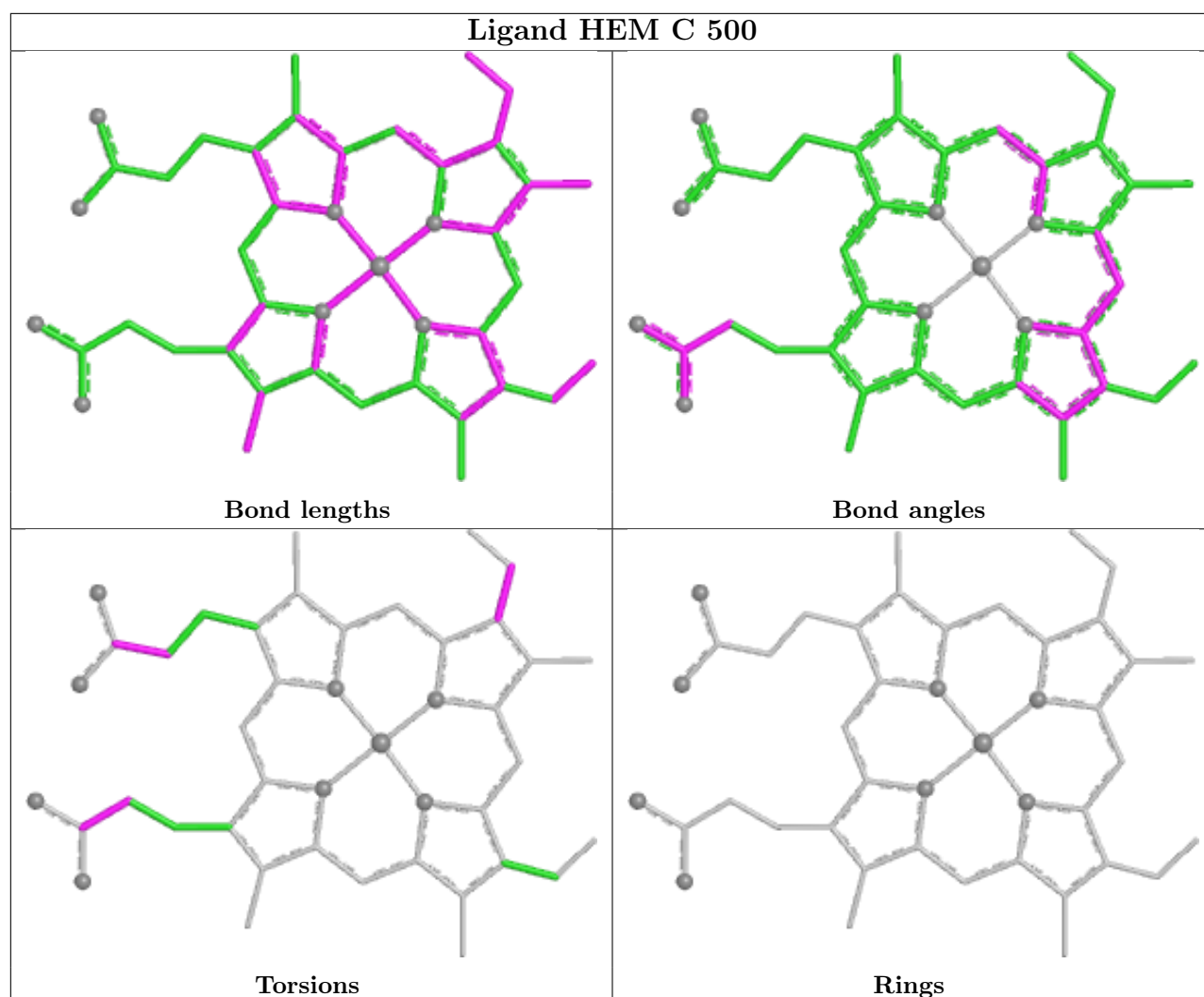
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	D1G	3	0
4	A	501	D1G	3	0
3	B	500	HEM	2	0
4	C	501	D1G	3	0
4	D	501	D1G	4	0
3	A	500	HEM	5	0
3	D	500	HEM	5	0
3	C	500	HEM	4	0

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	465/476 (97%)	0.85	31 (6%) 24 26	17, 28, 46, 66	0
1	B	463/476 (97%)	1.22	66 (14%) 6 6	20, 34, 55, 67	0
1	C	464/476 (97%)	0.62	22 (4%) 36 39	18, 28, 46, 65	0
1	D	464/476 (97%)	1.28	71 (15%) 5 5	18, 29, 55, 68	0
All	All	1856/1904 (97%)	0.99	190 (10%) 12 12	17, 30, 50, 68	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	31	GLY	5.9
1	D	140	VAL	5.5
1	C	31	GLY	5.5
1	D	139	GLY	5.0
1	B	258	THR	4.4
1	D	144	GLY	4.1
1	B	260	ASP	4.0
1	B	61	ILE	3.8
1	B	261	PRO	3.7
1	D	138	PHE	3.7
1	D	141	GLY	3.7
1	B	259	LEU	3.7
1	C	417	LEU	3.6
1	D	143	ARG	3.6
1	C	418	ASN	3.5
1	D	336	GLY	3.5
1	A	30	LYS	3.5
1	D	257	ARG	3.5
1	D	264	PRO	3.4
1	B	253	GLU	3.4
1	B	273	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	240	LEU	3.4
1	B	383	PHE	3.4
1	B	193	TYR	3.3
1	D	259	LEU	3.2
1	D	142	LYS	3.2
1	D	417	LEU	3.1
1	B	195	ASP	3.1
1	B	404	PHE	3.1
1	D	354	ALA	3.1
1	C	199	LEU	3.0
1	B	262	ASN	3.0
1	D	261	PRO	3.0
1	B	59	MET	3.0
1	C	159	ALA	3.0
1	A	260	ASP	2.9
1	B	208	ILE	2.9
1	D	421	GLY	2.9
1	D	493	PRO	2.9
1	A	262	ASN	2.9
1	D	422	GLN	2.9
1	B	457	MET	2.9
1	D	249	ALA	2.9
1	A	322	GLU	2.9
1	B	337	LYS	2.8
1	D	282	PRO	2.8
1	D	260	ASP	2.8
1	B	446	ARG	2.8
1	D	262	ASN	2.8
1	A	406	SER	2.7
1	B	53	GLN	2.7
1	D	255	ASN	2.7
1	D	432	PHE	2.7
1	C	421	GLY	2.7
1	B	64	ARG	2.7
1	B	65	TYR	2.7
1	C	325	ALA	2.7
1	D	271	PHE	2.7
1	C	160	LEU	2.7
1	B	282	PRO	2.7
1	A	208	ILE	2.7
1	B	143	ARG	2.7
1	D	32	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	254	HIS	2.7
1	D	83	GLY	2.7
1	A	383	PHE	2.7
1	B	468	PRO	2.7
1	D	331	ILE	2.7
1	C	336	GLY	2.6
1	D	457	MET	2.6
1	C	193	TYR	2.6
1	B	32	LYS	2.6
1	B	216	THR	2.6
1	B	338	ASN	2.6
1	D	404	PHE	2.6
1	A	257	ARG	2.6
1	B	382	ASP	2.6
1	D	420	LYS	2.6
1	B	63	GLU	2.6
1	C	161	ARG	2.5
1	C	282	PRO	2.5
1	D	145	ILE	2.5
1	B	403	SER	2.5
1	D	258	THR	2.5
1	A	259	LEU	2.5
1	A	263	SER	2.5
1	D	382	ASP	2.5
1	B	379	LYS	2.5
1	B	141	GLY	2.5
1	D	383	PHE	2.5
1	D	405	PHE	2.5
1	B	133	ALA	2.5
1	B	454	THR	2.5
1	B	68	VAL	2.5
1	A	264	PRO	2.5
1	A	336	GLY	2.4
1	B	336	GLY	2.4
1	B	264	PRO	2.4
1	D	188	GLY	2.4
1	D	135	LEU	2.4
1	D	273	ILE	2.4
1	B	60	LYS	2.4
1	D	250	LYS	2.4
1	A	271	PHE	2.4
1	D	384	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	37	PRO	2.4
1	D	275	MET	2.4
1	B	57	SER	2.4
1	A	189	ASP	2.3
1	D	494	ARG	2.3
1	B	423	PHE	2.3
1	B	422	GLN	2.3
1	A	421	GLY	2.3
1	C	461	ARG	2.3
1	A	247	PHE	2.3
1	B	384	PHE	2.3
1	D	416	PHE	2.3
1	B	168	ILE	2.3
1	D	195	ASP	2.3
1	C	147	GLU	2.3
1	B	272	LEU	2.3
1	B	288	LEU	2.3
1	A	32	LYS	2.3
1	B	138	PHE	2.3
1	D	187	PHE	2.3
1	D	31	GLY	2.3
1	D	256	GLN	2.3
1	A	255	ASN	2.3
1	D	60	LYS	2.3
1	D	124	ALA	2.2
1	D	380	PHE	2.2
1	D	435	GLY	2.2
1	A	382	ASP	2.2
1	B	492	LEU	2.2
1	C	419	GLU	2.2
1	D	33	LEU	2.2
1	A	261	PRO	2.2
1	B	421	GLY	2.2
1	B	287	TYR	2.2
1	A	273	ILE	2.2
1	B	254	HIS	2.2
1	D	263	SER	2.2
1	D	86	ALA	2.2
1	D	172	PHE	2.2
1	B	471	ILE	2.2
1	B	323	VAL	2.2
1	B	334	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	124	ALA	2.2
1	C	376	LYS	2.2
1	C	457	MET	2.1
1	A	147	GLU	2.1
1	B	269	ASP	2.1
1	A	139	GLY	2.1
1	C	412	ASN	2.1
1	C	335	ILE	2.1
1	D	287	TYR	2.1
1	A	270	SER	2.1
1	B	92	VAL	2.1
1	D	68	VAL	2.1
1	A	251	LYS	2.1
1	C	337	LYS	2.1
1	B	34	PRO	2.1
1	D	338	ASN	2.1
1	B	210	GLN	2.1
1	D	237	ALA	2.1
1	D	325	ALA	2.1
1	B	343	PHE	2.1
1	D	335	ILE	2.1
1	D	381	ARG	2.1
1	D	406	SER	2.1
1	D	464	SER	2.1
1	B	415	HIS	2.1
1	A	466	GLN	2.1
1	B	350	PRO	2.1
1	A	90	ALA	2.1
1	B	325	ALA	2.1
1	B	194	LYS	2.0
1	C	32	LYS	2.0
1	C	425	LYS	2.0
1	D	182	ILE	2.0
1	B	252	VAL	2.0
1	A	291	LEU	2.0
1	D	137	ASP	2.0
1	B	419	GLU	2.0
1	B	36	GLY	2.0
1	B	256	GLN	2.0
1	D	276	GLN	2.0
1	D	340	GLN	2.0
1	D	386	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	468	PRO	2.0

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

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

6.3 Carbohydrates [\(i\)](#)

There are no oligosaccharides in this entry.

6.4 Ligands [\(i\)](#)

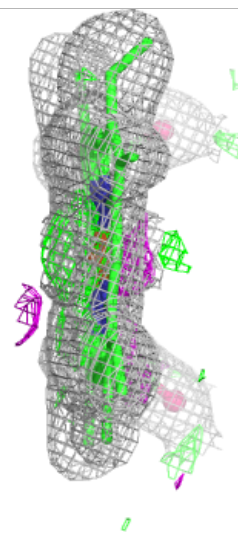
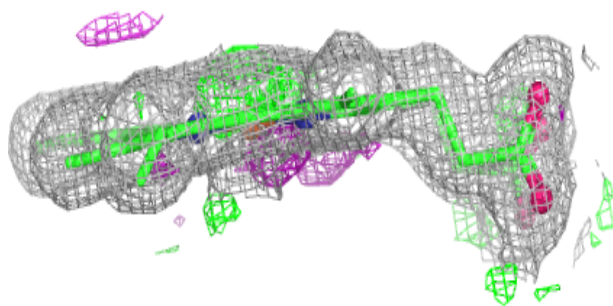
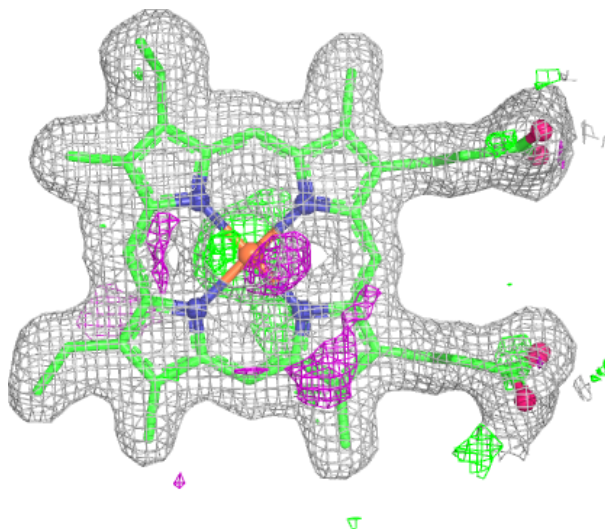
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	A	2502	5/5	0.77	0.11	61,62,64,67	0
2	SO4	A	2503	5/5	0.78	0.14	54,55,57,60	0
4	D1G	B	501	15/15	0.91	0.10	30,34,36,36	0
4	D1G	D	501	15/15	0.91	0.11	29,34,35,35	0
4	D1G	A	501	15/15	0.92	0.09	23,27,30,30	0
3	HEM	D	500	43/43	0.93	0.12	17,21,23,30	0
4	D1G	C	501	15/15	0.94	0.10	29,31,35,35	0
3	HEM	B	500	43/43	0.96	0.08	19,24,27,31	0
3	HEM	A	500	43/43	0.96	0.08	17,19,22,26	0
3	HEM	C	500	43/43	0.97	0.07	18,22,24,26	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.

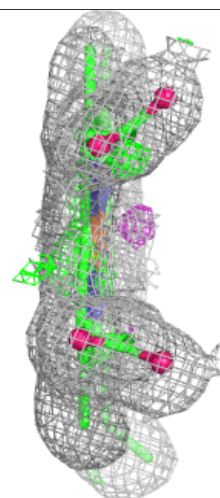
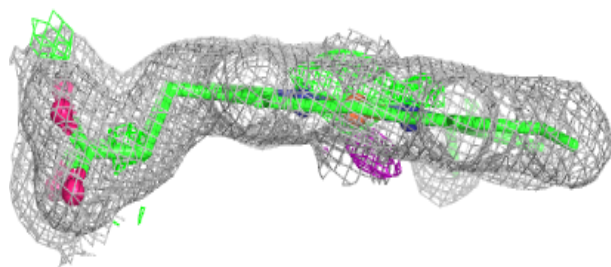
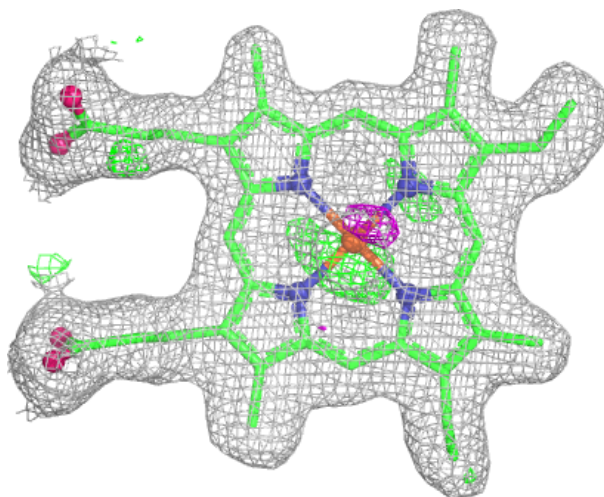
Electron density around HEM D 500:

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



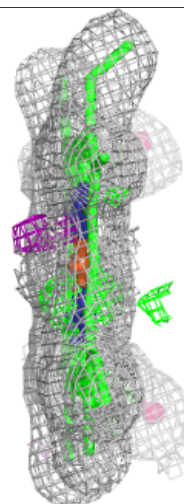
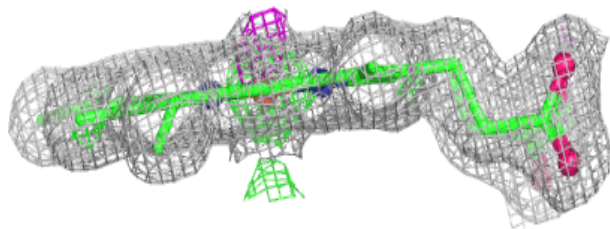
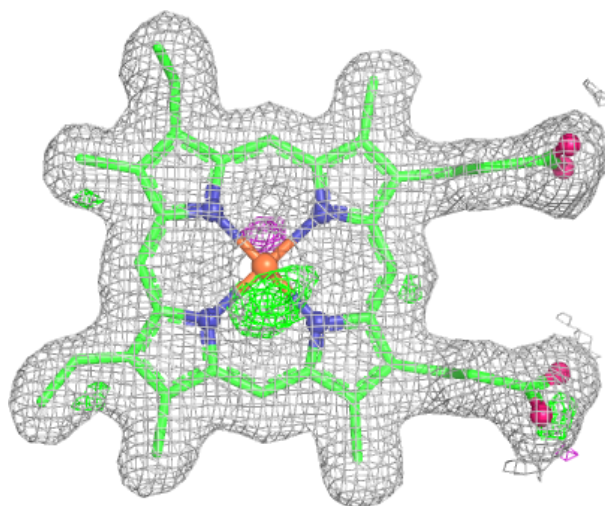
Electron density around HEM B 500:

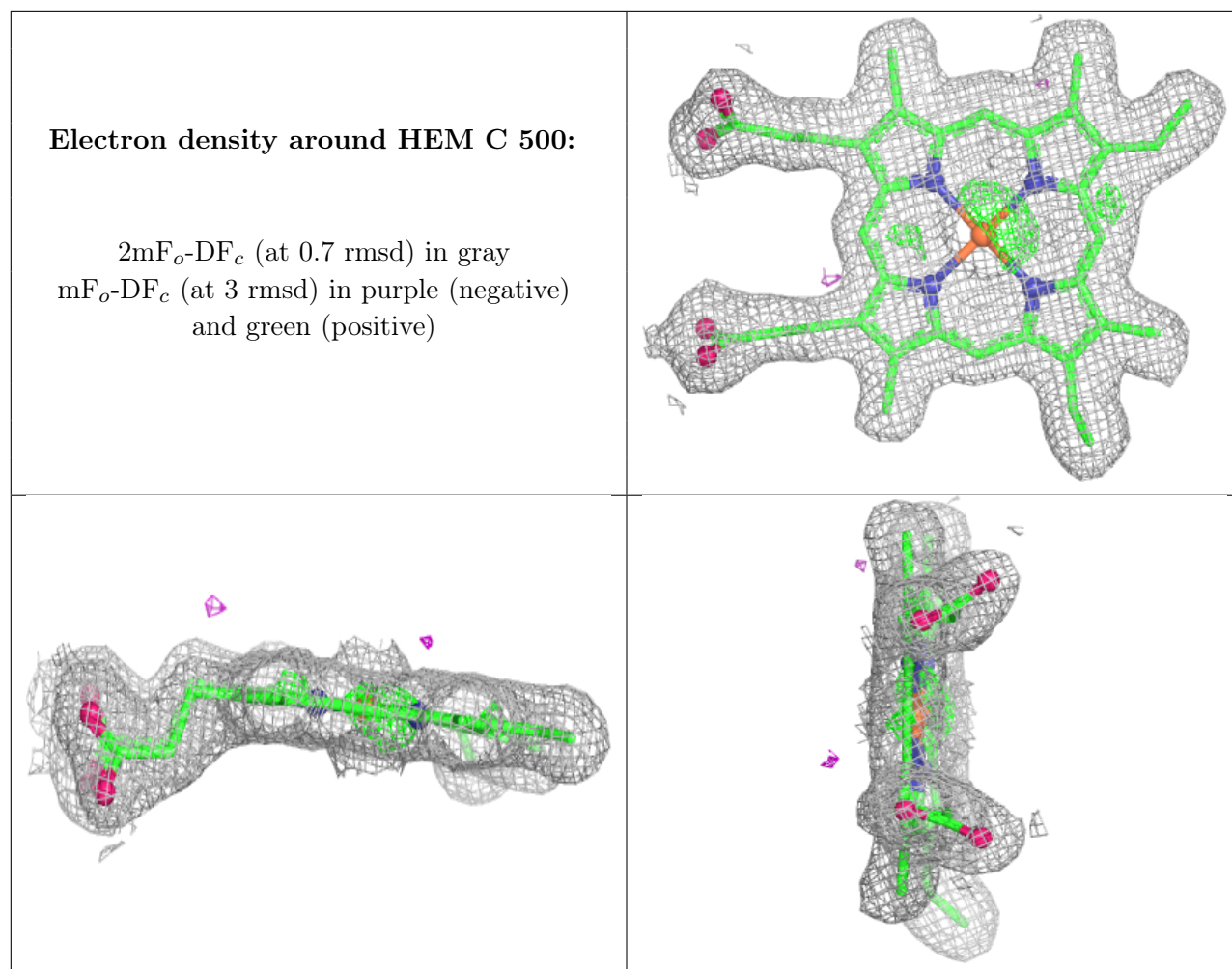
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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 [i](#)

There are no such residues in this entry.