



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:55 AM UTC

PDB ID : 1PQ2 / pdb_00001pq2
Title : Crystal Structure of Human Drug Metabolizing Cytochrome P450 2C8
Authors : Schoch, G.A.; Yano, J.K.; Wester, M.R.; Griffin, K.J.; Stout, C.D.; Johnson, E.F.
Deposited on : 2003-06-17
Resolution : 2.70 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)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

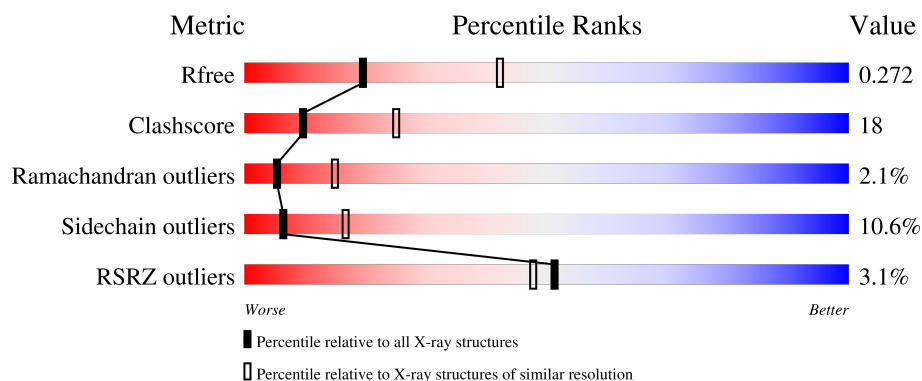
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	3% 59% 29% 7% • •
1	B	476	4% 58% 32% 7% • •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7550 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 2C8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	0	0
			3693	2362	635	674	22			
1	B	463	Total	C	N	O	S	0	0	0
			3693	2362	635	674	22			

There are 26 discrepancies between the modelled and reference sequences:

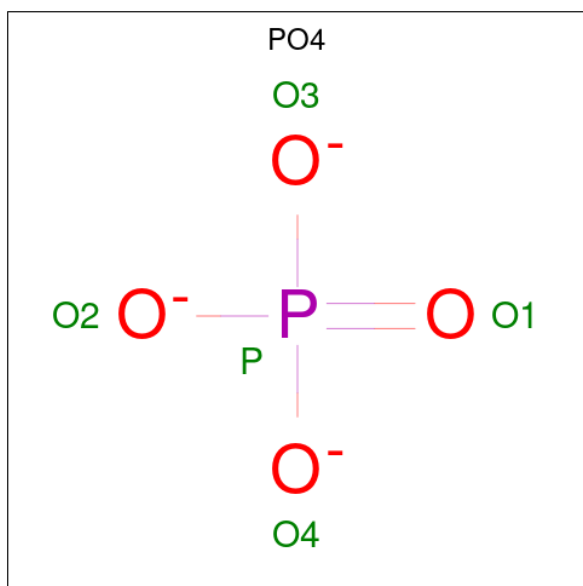
Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	engineered mutation	UNP P10632
A	20	ALA	-	engineered mutation	UNP P10632
A	21	LYS	-	engineered mutation	UNP P10632
A	22	LYS	-	engineered mutation	UNP P10632
A	23	THR	-	engineered mutation	UNP P10632
A	24	SER	-	engineered mutation	UNP P10632
A	25	SER	-	engineered mutation	UNP P10632
A	26	LYS	-	engineered mutation	UNP P10632
A	27	GLY	-	engineered mutation	UNP P10632
A	491	HIS	-	expression tag	UNP P10632
A	492	HIS	-	expression tag	UNP P10632
A	493	HIS	-	expression tag	UNP P10632
A	494	HIS	-	expression tag	UNP P10632
B	19	MET	-	engineered mutation	UNP P10632
B	20	ALA	-	engineered mutation	UNP P10632
B	21	LYS	-	engineered mutation	UNP P10632
B	22	LYS	-	engineered mutation	UNP P10632
B	23	THR	-	engineered mutation	UNP P10632
B	24	SER	-	engineered mutation	UNP P10632
B	25	SER	-	engineered mutation	UNP P10632
B	26	LYS	-	engineered mutation	UNP P10632
B	27	GLY	-	engineered mutation	UNP P10632
B	491	HIS	-	expression tag	UNP P10632
B	492	HIS	-	expression tag	UNP P10632
B	493	HIS	-	expression tag	UNP P10632

Continued on next page...

Continued from previous page...

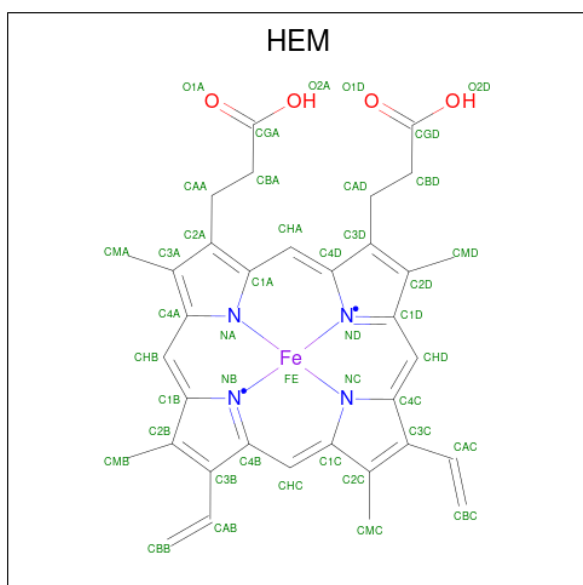
Chain	Residue	Modelled	Actual	Comment	Reference
B	494	HIS	-	expression tag	UNP P10632

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



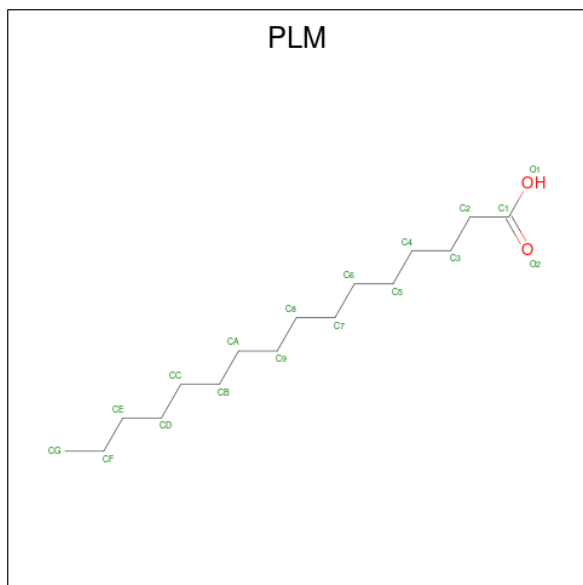
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		

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



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

- Molecule 4 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O		
			18	16	2	0	0
4	B	1	Total	C	O		
			18	16	2	0	0

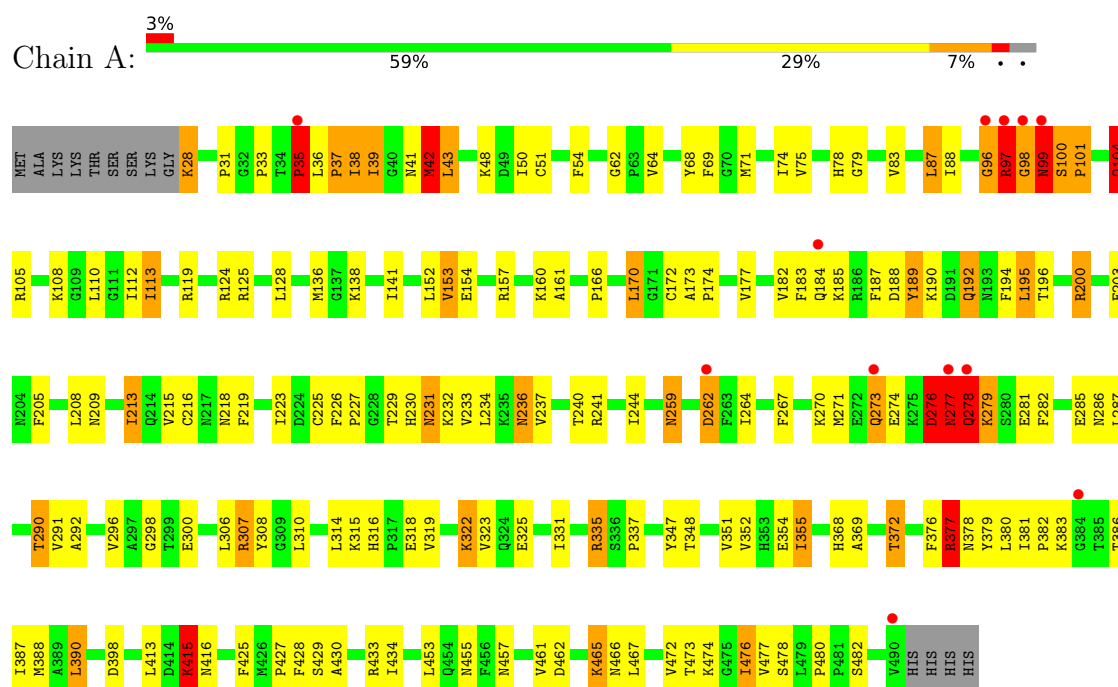
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	22	Total	O		
			22	22	0	0
5	B	15	Total	O		
			15	15	0	0

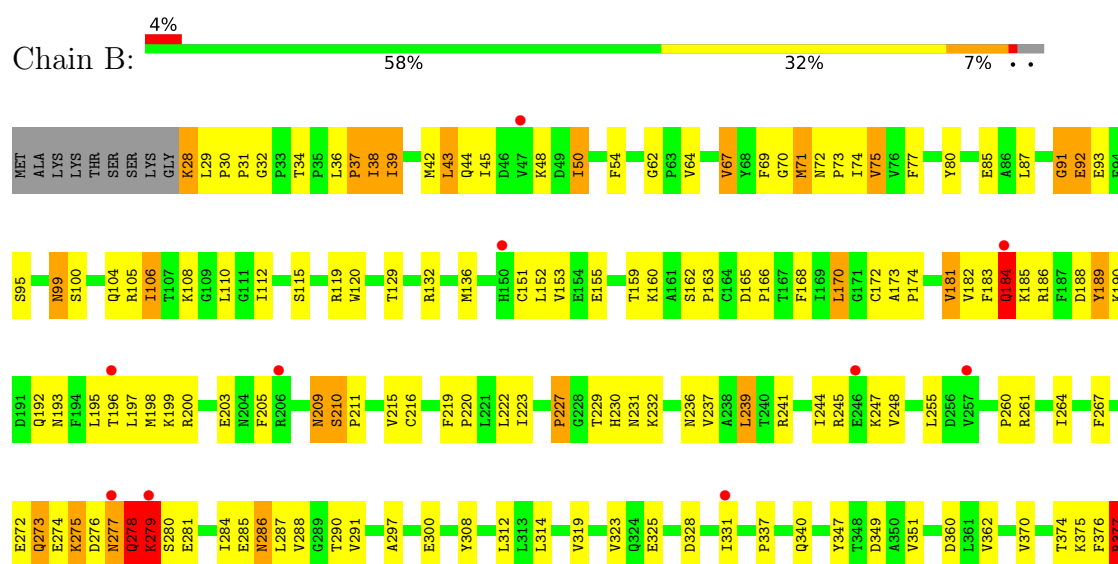
3 Residue-property plots [i](#)

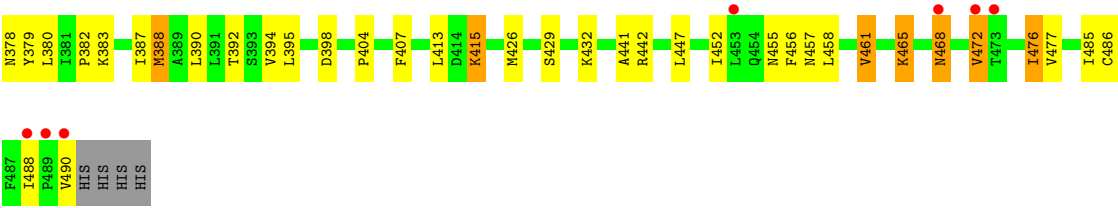
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 2C8



• Molecule 1: Cytochrome P450 2C8





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.99Å 137.41Å 97.32Å 90.00° 112.51° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.8 (50.00-2.70) 97.8 (50.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.248 , 0.288 0.233 , 0.272	Depositor DCC
R_{free} test set	1937 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	61.8	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7550	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, PLM, PO4

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	0.64	8/3778 (0.2%)	1.22	36/5115 (0.7%)
1	B	0.55	1/3778 (0.0%)	1.10	35/5115 (0.7%)
All	All	0.59	9/7556 (0.1%)	1.16	71/10230 (0.7%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	GLY	CA-C	-9.70	1.44	1.51
1	A	99	ASN	N-CA	-6.90	1.37	1.46
1	A	98	GLY	C-N	-6.43	1.25	1.33
1	A	97	ARG	N-CA	-5.55	1.39	1.46
1	A	99	ASN	CA-C	-5.38	1.46	1.52
1	B	37	PRO	N-CA	5.28	1.54	1.47
1	A	97	ARG	CA-C	-5.22	1.45	1.52
1	A	96	GLY	C-N	-5.18	1.27	1.33
1	A	97	ARG	C-N	-5.09	1.31	1.33

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	PRO	CA-N-CD	-14.98	91.03	112.00
1	A	101	PRO	CA-N-CD	-11.78	95.51	112.00
1	A	62	GLY	CA-C-N	11.10	130.79	119.24
1	A	62	GLY	C-N-CA	11.10	130.79	119.24
1	A	273	GLN	OE1-CD-NE2	-10.09	112.51	122.60
1	A	104	GLN	OE1-CD-NE2	-9.82	112.78	122.60
1	A	276	ASP	CA-CB-CG	9.81	122.41	112.60
1	B	273	GLN	OE1-CD-NE2	-9.72	112.88	122.60
1	A	278	GLN	OE1-CD-NE2	-9.49	113.11	122.60
1	B	184	GLN	OE1-CD-NE2	-9.43	113.17	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	278	GLN	OE1-CD-NE2	-9.41	113.19	122.60
1	B	37	PRO	N-CA-C	9.40	131.83	112.47
1	A	98	GLY	CA-C-N	-8.20	108.56	122.33
1	A	98	GLY	C-N-CA	-8.20	108.56	122.33
1	B	62	GLY	CA-C-N	7.32	126.59	118.97
1	B	62	GLY	C-N-CA	7.32	126.59	118.97
1	A	99	ASN	CA-CB-CG	-7.27	105.33	112.60
1	A	306	LEU	N-CA-C	-7.17	103.46	111.28
1	B	37	PRO	CA-N-CD	-7.14	102.00	112.00
1	A	316	HIS	CA-C-N	7.13	126.39	118.97
1	A	316	HIS	C-N-CA	7.13	126.39	118.97
1	A	276	ASP	CA-C-N	7.13	135.15	121.54
1	A	276	ASP	C-N-CA	7.13	135.15	121.54
1	A	273	GLN	CG-CD-NE2	7.12	127.08	116.40
1	B	277	ASN	N-CA-C	-6.99	105.37	114.04
1	B	184	GLN	CG-CD-NE2	6.97	126.86	116.40
1	A	277	ASN	N-CA-C	6.83	125.35	110.80
1	B	70	GLY	N-CA-C	-6.77	97.14	113.18
1	A	278	GLN	CG-CD-NE2	6.75	126.52	116.40
1	A	37	PRO	N-CA-C	6.70	126.28	112.47
1	A	104	GLN	CG-CD-NE2	6.66	126.39	116.40
1	B	273	GLN	CG-CD-NE2	6.65	126.37	116.40
1	B	71	MET	N-CA-C	-6.55	104.92	113.17
1	B	165	ASP	CA-C-N	6.50	126.19	119.82
1	B	165	ASP	C-N-CA	6.50	126.19	119.82
1	B	278	GLN	CG-CD-NE2	6.45	126.07	116.40
1	B	362	VAL	CA-C-N	6.22	127.61	119.84
1	B	362	VAL	C-N-CA	6.22	127.61	119.84
1	A	99	ASN	CA-C-N	6.14	132.43	122.48
1	A	99	ASN	C-N-CA	6.14	132.43	122.48
1	A	99	ASN	CA-C-O	6.12	127.81	120.28
1	A	390	LEU	N-CA-C	6.12	119.16	108.52
1	B	91	GLY	N-CA-C	6.01	121.27	113.27
1	A	96	GLY	N-CA-C	-5.96	102.84	112.31
1	A	195	LEU	N-CA-C	5.88	117.76	111.36
1	A	112	ILE	CB-CA-C	-5.76	105.93	111.05
1	B	36	LEU	N-CA-C	-5.74	102.42	109.65
1	B	297	ALA	N-CA-C	5.71	119.97	112.89
1	B	210	SER	CA-C-N	5.69	125.37	119.56
1	B	210	SER	C-N-CA	5.69	125.37	119.56
1	B	398	ASP	N-CA-C	5.66	117.25	111.14
1	B	37	PRO	N-CA-CB	-5.46	97.52	103.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	255	LEU	N-CA-C	5.46	118.14	109.96
1	B	32	GLY	CA-C-N	5.45	125.76	119.93
1	B	32	GLY	C-N-CA	5.45	125.76	119.93
1	B	456	PHE	N-CA-C	5.45	118.39	110.17
1	A	87	LEU	N-CA-C	5.32	118.94	112.23
1	B	34	THR	CA-C-N	5.25	125.65	119.99
1	B	34	THR	C-N-CA	5.25	125.65	119.99
1	B	488	ILE	N-CA-C	5.23	113.62	107.77
1	B	230	HIS	N-CA-C	-5.22	104.84	111.11
1	A	37	PRO	CA-N-CD	-5.15	104.79	112.00
1	B	219	PHE	CA-C-N	5.14	126.27	119.84
1	B	219	PHE	C-N-CA	5.14	126.27	119.84
1	A	100	SER	N-CA-C	5.12	116.02	110.13
1	A	262	ASP	N-CA-C	5.08	114.85	108.45
1	A	96	GLY	O-C-N	5.08	127.18	122.81
1	A	355	ILE	N-CA-C	-5.07	105.77	110.53
1	B	349	ASP	N-CA-C	-5.06	105.84	111.36
1	A	113	ILE	CB-CA-C	-5.06	105.40	111.88
1	A	457	ASN	N-CA-C	-5.03	101.90	109.85

There are no chirality outliers.

There are no planarity outliers.

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	3693	0	3715	135	0
1	B	3693	0	3715	132	0
2	A	5	0	0	0	0
3	A	43	0	30	2	0
3	B	43	0	30	2	0
4	A	18	0	31	3	0
4	B	18	0	31	6	0
5	A	22	0	0	0	0
5	B	15	0	0	0	0
All	All	7550	0	7552	266	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 18.

All (266) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:GLU:HG2	1:B:376:PHE:CE1	1.93	1.03
1:A:35:PRO:HD3	1:A:41:ASN:HD21	1.22	1.00
1:B:278:GLN:HG2	1:B:279:LYS:H	1.34	0.93
1:A:105:ARG:HD2	4:B:501:PLM:HG3	1.51	0.92
1:A:209:ASN:HD22	1:A:476:ILE:HD13	1.35	0.90
1:A:35:PRO:HD3	1:A:41:ASN:ND2	1.89	0.88
1:B:209:ASN:HD22	1:B:476:ILE:HD13	1.41	0.85
1:B:43:LEU:HD12	1:B:43:LEU:H	1.41	0.85
1:B:415:LYS:HD3	1:B:415:LYS:H	1.40	0.85
1:A:307:ARG:HH21	1:A:307:ARG:HG3	1.43	0.81
1:A:98:GLY:O	1:A:99:ASN:ND2	2.13	0.81
1:B:468:ASN:H	1:B:468:ASN:HD22	1.25	0.81
1:B:151:CYS:SG	1:B:186:ARG:NH1	2.54	0.80
1:A:33:PRO:O	1:A:35:PRO:HD2	1.81	0.80
1:A:229:THR:HG21	4:B:501:PLM:H61	1.64	0.80
1:A:43:LEU:H	1:A:43:LEU:HD12	1.48	0.79
1:B:377:ARG:O	1:B:378:ASN:HB2	1.83	0.78
1:B:110:LEU:HD23	1:B:119:ARG:HH22	1.47	0.78
1:A:28:LYS:NZ	1:A:28:LYS:HA	2.01	0.76
1:B:119:ARG:HA	1:B:281:GLU:HG3	1.67	0.76
1:B:172:CYS:SG	1:B:198:MET:HE1	2.26	0.75
1:B:184:GLN:O	1:B:184:GLN:HG2	1.86	0.75
1:B:39:ILE:HG13	1:B:43:LEU:HD11	1.68	0.75
1:A:42:MET:HE2	1:A:219:PHE:HE1	1.52	0.74
1:B:286:ASN:O	1:B:290:THR:HG22	1.88	0.74
1:A:97:ARG:CD	1:A:113:ILE:O	2.37	0.73
1:B:85:GLU:HG2	1:B:376:PHE:HE1	1.50	0.73
1:A:209:ASN:HD21	1:A:477:VAL:H	1.38	0.72
1:B:110:LEU:HD23	1:B:119:ARG:NH2	2.04	0.72
1:B:465:LYS:HE3	1:B:465:LYS:HA	1.71	0.71
1:A:173:ALA:HB3	1:A:174:PRO:HD3	1.72	0.70
1:B:173:ALA:HB3	1:B:174:PRO:HD3	1.75	0.68
1:A:96:GLY:HA3	1:A:369:ALA:O	1.94	0.67
1:B:278:GLN:HG2	1:B:279:LYS:N	2.07	0.67
1:A:183:PHE:O	1:A:184:GLN:HG3	1.94	0.67
1:A:259:ASN:H	1:A:259:ASN:HD22	1.41	0.67
1:A:97:ARG:HD3	1:A:113:ILE:O	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:VAL:HG11	1:B:291:VAL:HG13	1.77	0.66
1:A:192:GLN:HE21	1:A:192:GLN:HA	1.61	0.66
1:A:35:PRO:HG2	1:A:68:TYR:CD1	2.32	0.65
1:A:192:GLN:HA	1:A:192:GLN:NE2	2.12	0.64
1:B:267:PHE:CE2	1:B:287:LEU:HB2	2.33	0.64
1:A:157:ARG:HG3	1:A:157:ARG:HH11	1.63	0.64
1:A:153:VAL:HG11	1:A:455:ASN:HD22	1.63	0.63
1:B:50:ILE:HD13	1:B:50:ILE:O	1.99	0.63
1:A:209:ASN:ND2	1:A:476:ILE:HD13	2.11	0.63
1:A:425:PHE:CZ	1:A:427:PRO:HG3	2.33	0.63
1:B:77:PHE:HE2	1:B:387:ILE:HD12	1.63	0.62
1:B:168:PHE:HZ	1:B:195:LEU:HD12	1.64	0.62
1:A:185:LYS:HD2	1:A:185:LYS:O	1.99	0.62
1:B:272:GLU:O	1:B:275:LYS:HG3	1.99	0.62
1:A:170:LEU:HD21	1:A:310:LEU:HD12	1.81	0.62
1:A:69:PHE:CD2	1:A:74:ILE:HD12	2.34	0.61
1:B:39:ILE:HD13	1:B:39:ILE:H	1.64	0.61
1:A:259:ASN:HD22	1:A:259:ASN:N	1.98	0.60
1:B:185:LYS:HD2	1:B:185:LYS:O	2.01	0.60
1:A:331:ILE:HG23	1:A:335:ARG:HE	1.66	0.60
1:B:267:PHE:CG	1:B:287:LEU:HD13	2.36	0.60
1:B:241:ARG:O	1:B:245:ARG:HG2	2.01	0.60
1:B:93:GLU:O	1:B:370:VAL:HA	2.01	0.60
1:A:205:PHE:CD1	1:A:300:GLU:HG2	2.37	0.59
1:B:209:ASN:HD22	1:B:476:ILE:CD1	2.13	0.59
1:B:39:ILE:O	1:B:42:MET:HB2	2.02	0.59
1:B:28:LYS:HA	1:B:28:LYS:NZ	2.17	0.59
1:A:38:ILE:HG13	1:A:71:MET:HE1	1.84	0.59
1:B:29:LEU:HD21	1:B:382:PRO:HD2	1.85	0.58
1:B:205:PHE:CD1	1:B:300:GLU:HG2	2.38	0.58
1:A:64:VAL:HG21	1:A:376:PHE:CE2	2.39	0.58
1:B:216:CYS:HB3	1:B:223:ILE:HD13	1.86	0.58
1:A:39:ILE:HD13	1:A:39:ILE:H	1.69	0.57
1:A:119:ARG:HA	1:A:281:GLU:HG3	1.85	0.57
1:B:38:ILE:HG22	1:B:39:ILE:HG23	1.86	0.57
1:B:277:ASN:O	1:B:279:LYS:N	2.37	0.56
4:A:502:PLM:HG3	1:B:105:ARG:HD2	1.85	0.56
1:A:43:LEU:HD12	1:A:43:LEU:N	2.18	0.56
1:A:237:VAL:O	1:A:241:ARG:HG3	2.05	0.56
1:B:209:ASN:ND2	1:B:476:ILE:HD13	2.15	0.56
1:A:331:ILE:HD13	1:A:337:PRO:HB3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ARG:HD2	1:A:286:ASN:HD21	1.70	0.56
1:A:473:THR:HG23	1:A:478:SER:HB3	1.87	0.56
1:A:192:GLN:HE21	1:A:192:GLN:CA	2.18	0.56
1:B:248:VAL:HG22	1:B:264:ILE:HD12	1.87	0.56
1:A:192:GLN:O	1:A:196:THR:HG23	2.06	0.55
1:A:28:LYS:HA	1:A:28:LYS:HZ1	1.71	0.55
1:B:106:ILE:HG23	1:B:237:VAL:HG21	1.88	0.55
1:A:33:PRO:O	1:A:35:PRO:CD	2.54	0.55
1:A:136:MET:HE2	1:A:141:ILE:HG12	1.89	0.55
1:A:182:VAL:HG11	1:A:291:VAL:HG13	1.88	0.55
1:A:75:VAL:CG1	1:A:387:ILE:HD13	2.36	0.55
1:A:415:LYS:H	1:A:415:LYS:HD3	1.71	0.55
1:A:287:LEU:O	1:A:290:THR:HG22	2.07	0.55
1:A:64:VAL:HG21	1:A:376:PHE:HE2	1.71	0.54
1:A:348:THR:O	1:A:352:VAL:HG23	2.07	0.54
1:A:229:THR:HG21	4:B:501:PLM:H81	1.88	0.54
1:B:360:ASP:OD2	1:B:392:THR:HG23	2.07	0.54
1:B:376:PHE:CD2	1:B:377:ARG:HG2	2.41	0.54
1:B:54:PHE:HB3	1:B:390:LEU:HD11	1.90	0.54
1:A:229:THR:CG2	4:B:501:PLM:H81	2.38	0.54
1:A:307:ARG:HE	1:A:480:PRO:HG2	1.73	0.54
1:B:277:ASN:O	1:B:278:GLN:HG2	2.07	0.54
1:A:189:TYR:O	1:A:195:LEU:HD21	2.08	0.54
1:A:229:THR:O	1:A:233:VAL:HG23	2.09	0.53
1:A:97:ARG:HB3	1:A:433:ARG:NH1	2.24	0.53
1:B:188:ASP:C	1:B:190:LYS:H	2.16	0.53
1:A:152:LEU:HD13	1:A:173:ALA:HB2	1.90	0.53
1:A:351:VAL:O	1:A:355:ILE:HG13	2.08	0.53
1:A:415:LYS:H	1:A:415:LYS:CD	2.21	0.53
1:B:216:CYS:HB3	1:B:223:ILE:CD1	2.38	0.53
1:A:307:ARG:HG3	1:A:307:ARG:NH2	2.17	0.52
1:A:368:HIS:HB2	1:A:387:ILE:HB	1.92	0.52
1:A:216:CYS:HB3	1:A:223:ILE:HD13	1.90	0.52
1:A:200:ARG:HG3	1:A:236:ASN:ND2	2.25	0.52
1:B:99:ASN:C	1:B:99:ASN:HD22	2.17	0.52
1:B:244:ILE:HB	1:B:288:VAL:HG13	1.92	0.52
1:A:184:GLN:HB3	1:A:262:ASP:HB3	1.92	0.52
1:A:33:PRO:HB2	1:A:41:ASN:ND2	2.25	0.52
1:B:284:ILE:O	1:B:288:VAL:HG23	2.09	0.52
1:B:200:ARG:NH1	1:B:239:LEU:HD12	2.25	0.52
1:B:319:VAL:HG13	1:B:347:TYR:OH	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ILE:HD11	1:A:430:ALA:HB1	1.92	0.52
1:B:472:VAL:HG22	1:B:472:VAL:O	2.10	0.52
1:A:234:LEU:HG	4:B:501:PLM:HG2	1.93	0.51
1:B:182:VAL:HG11	1:B:291:VAL:CG1	2.39	0.51
1:A:298:GLY:HA2	3:A:500:HEM:C2C	2.45	0.51
1:A:461:VAL:HG12	1:A:461:VAL:O	2.10	0.51
1:B:28:LYS:HA	1:B:28:LYS:HZ3	1.73	0.51
1:A:42:MET:HE2	1:A:219:PHE:CE1	2.40	0.51
1:A:227:PRO:O	1:A:231:ASN:HB2	2.11	0.51
1:A:216:CYS:HB3	1:A:223:ILE:CD1	2.41	0.50
1:B:184:GLN:O	1:B:184:GLN:CG	2.58	0.50
4:A:502:PLM:HA2	1:B:223:ILE:HD12	1.94	0.50
1:B:119:ARG:HD3	1:B:286:ASN:HD21	1.76	0.50
1:B:153:VAL:HG11	1:B:455:ASN:ND2	2.25	0.49
1:B:370:VAL:HG23	1:B:383:LYS:HA	1.94	0.49
1:B:458:LEU:HD22	1:B:485:ILE:HD11	1.94	0.49
1:B:183:PHE:CE1	1:B:247:LYS:HG2	2.47	0.49
1:B:331:ILE:HD13	1:B:337:PRO:HB3	1.95	0.49
1:B:278:GLN:O	1:B:280:SER:N	2.46	0.49
1:A:292:ALA:O	1:A:296:VAL:HG23	2.13	0.48
1:B:319:VAL:O	1:B:323:VAL:HG23	2.12	0.48
1:A:476:ILE:HG12	1:A:477:VAL:HG23	1.95	0.48
1:B:129:THR:HA	1:B:132:ARG:HD3	1.96	0.48
1:A:271:MET:HG2	1:A:282:PHE:O	2.12	0.48
1:B:387:ILE:HG22	1:B:388:MET:N	2.27	0.48
1:A:183:PHE:HB3	1:A:185:LYS:HE3	1.95	0.48
1:A:315:LYS:HB2	1:A:467:LEU:HD23	1.95	0.48
1:B:395:LEU:HD21	1:B:426:MET:H	1.78	0.48
1:B:43:LEU:HD12	1:B:43:LEU:N	2.20	0.48
1:B:168:PHE:HZ	1:B:195:LEU:CD1	2.26	0.48
1:A:428:PHE:O	1:A:429:SER:HB3	2.14	0.48
1:A:174:PRO:O	1:A:177:VAL:HB	2.13	0.47
1:A:36:LEU:N	1:A:36:LEU:HD12	2.29	0.47
1:B:184:GLN:OE1	1:B:261:ARG:HB3	2.15	0.47
1:B:415:LYS:H	1:B:415:LYS:CD	2.11	0.47
1:B:159:THR:O	1:B:162:SER:HB3	2.14	0.47
1:A:354:GLU:O	1:A:354:GLU:HG3	2.15	0.46
1:B:199:LYS:O	1:B:203:GLU:HG3	2.15	0.46
1:B:136:MET:O	1:B:260:PRO:HB2	2.16	0.46
1:A:153:VAL:HG11	1:A:455:ASN:ND2	2.29	0.46
1:A:188:ASP:O	1:A:190:LYS:N	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:ILE:HG12	1:B:477:VAL:HG23	1.98	0.46
1:A:240:THR:O	1:A:244:ILE:HG13	2.16	0.46
1:A:31:PRO:HD3	1:A:379:TYR:CE2	2.51	0.46
1:A:97:ARG:HD2	1:A:113:ILE:O	2.13	0.46
1:A:28:LYS:HA	1:A:28:LYS:HZ2	1.77	0.46
1:B:92:GLU:HG2	1:B:432:LYS:HE2	1.98	0.46
1:B:376:PHE:O	1:B:377:ARG:C	2.59	0.45
1:B:429:SER:CB	3:B:500:HEM:HBA1	2.47	0.45
1:B:75:VAL:HG22	1:B:77:PHE:CE2	2.52	0.45
1:B:220:PRO:O	1:B:223:ILE:HG12	2.17	0.45
1:A:377:ARG:O	1:A:378:ASN:HB2	2.16	0.45
1:A:415:LYS:C	1:A:416:ASN:HD22	2.24	0.45
1:B:71:MET:HE2	1:B:71:MET:HB2	1.83	0.45
1:A:69:PHE:HB3	1:A:218:ASN:CG	2.42	0.45
1:A:322:LYS:HE3	1:A:322:LYS:HB2	1.77	0.45
1:A:226:PHE:N	1:A:227:PRO:HD3	2.32	0.45
1:A:267:PHE:CG	1:A:287:LEU:HD13	2.50	0.45
1:A:278:GLN:OE1	1:A:278:GLN:O	2.35	0.45
1:B:108:LYS:HG3	1:B:241:ARG:HH22	1.82	0.45
1:A:205:PHE:CG	1:A:300:GLU:HG2	2.53	0.44
1:A:54:PHE:HD2	1:A:390:LEU:HD11	1.83	0.44
1:B:195:LEU:HD22	1:B:195:LEU:H	1.82	0.44
1:B:192:GLN:O	1:B:196:THR:HG22	2.17	0.44
1:A:74:ILE:HG12	1:A:386:THR:CG2	2.46	0.44
1:B:91:GLY:O	1:B:95:SER:HB3	2.17	0.44
1:A:318:GLU:HG2	1:A:319:VAL:N	2.32	0.44
1:A:465:LYS:HE3	1:A:465:LYS:HA	2.00	0.44
1:B:45:ILE:HD11	1:B:67:VAL:HG21	2.00	0.44
1:A:187:PHE:HB3	1:A:194:PHE:HB2	2.00	0.44
4:A:502:PLM:H61	1:B:229:THR:HG21	2.00	0.44
1:A:79:GLY:O	1:A:83:VAL:HG23	2.17	0.44
1:B:115:SER:C	1:B:120:TRP:HB2	2.43	0.44
1:B:347:TYR:O	1:B:351:VAL:HG23	2.17	0.44
1:A:71:MET:HE2	1:A:71:MET:HB2	1.91	0.44
1:A:308:TYR:CD1	1:A:480:PRO:HB3	2.52	0.44
1:B:387:ILE:CG2	1:B:388:MET:N	2.79	0.44
1:A:166:PRO:O	1:A:170:LEU:HB2	2.18	0.44
1:B:209:ASN:HD21	1:B:477:VAL:H	1.65	0.44
1:A:138:LYS:N	1:A:138:LYS:HD2	2.33	0.43
1:A:203:GLU:OE2	1:A:232:LYS:HE2	2.18	0.43
1:A:157:ARG:HG3	1:A:157:ARG:NH1	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:PHE:CD2	1:B:74:ILE:HD12	2.53	0.43
1:B:159:THR:O	1:B:160:LYS:HB2	2.18	0.43
1:B:196:THR:HG23	1:B:197:LEU:N	2.33	0.43
1:B:468:ASN:H	1:B:468:ASN:ND2	2.02	0.43
1:B:490:VAL:HG12	1:B:490:VAL:O	2.19	0.43
1:A:208:LEU:HA	1:A:213:ILE:HG21	2.01	0.43
1:B:181:VAL:O	1:B:181:VAL:CG1	2.66	0.43
1:A:183:PHE:O	1:A:185:LYS:HG3	2.18	0.43
1:B:236:ASN:HD22	1:B:236:ASN:N	2.17	0.43
1:B:186:ARG:NH2	1:B:188:ASP:HA	2.34	0.43
1:B:28:LYS:O	1:B:379:TYR:HB3	2.19	0.43
1:B:287:LEU:O	1:B:291:VAL:HG23	2.19	0.43
1:B:110:LEU:CD1	1:B:285:GLU:HG3	2.48	0.42
1:B:54:PHE:HE1	1:B:67:VAL:HG11	1.85	0.42
1:B:312:LEU:HD13	1:B:407:PHE:CE1	2.54	0.42
1:A:38:ILE:CG1	1:A:71:MET:HE1	2.49	0.42
1:A:172:CYS:HB3	1:A:189:TYR:CE2	2.54	0.42
1:B:163:PRO:HB3	1:B:486:CYS:SG	2.59	0.42
1:A:259:ASN:N	1:A:259:ASN:ND2	2.67	0.42
1:B:166:PRO:O	1:B:170:LEU:HB2	2.18	0.42
1:B:274:GLU:O	1:B:275:LYS:C	2.61	0.42
1:A:225:CYS:C	1:A:227:PRO:HD3	2.45	0.42
1:A:276:ASP:CG	1:A:277:ASN:H	2.27	0.42
1:B:72:ASN:HA	1:B:73:PRO:HD2	1.93	0.42
1:B:375:LYS:HZ3	1:B:380:LEU:HD12	1.83	0.42
1:A:376:PHE:O	1:A:377:ARG:C	2.62	0.42
1:B:152:LEU:HD21	1:B:452:ILE:HD11	2.02	0.42
1:B:387:ILE:HD13	1:B:387:ILE:HA	1.88	0.42
1:A:372:THR:HA	1:A:383:LYS:HB2	2.00	0.42
1:A:78:HIS:ND1	1:A:78:HIS:C	2.78	0.41
1:B:110:LEU:HD13	1:B:285:GLU:HG3	2.02	0.41
1:B:31:PRO:HD3	1:B:379:TYR:CE2	2.55	0.41
1:B:69:PHE:CE2	1:B:74:ILE:HD12	2.55	0.41
1:B:441:ALA:HB1	3:B:500:HEM:HAB	2.02	0.41
1:B:468:ASN:HD22	1:B:468:ASN:N	2.02	0.41
1:A:474:LYS:HE2	1:B:227:PRO:HG2	2.01	0.41
1:B:155:GLU:HG3	1:B:189:TYR:CD1	2.54	0.41
1:B:457:ASN:OD1	1:B:490:VAL:HG21	2.20	0.41
1:A:347:TYR:O	1:A:351:VAL:HG23	2.20	0.41
1:A:110:LEU:HD11	1:A:285:GLU:HG3	2.02	0.41
1:A:154:GLU:O	1:A:157:ARG:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:LYS:HD3	1:B:415:LYS:N	2.21	0.41
1:A:97:ARG:CB	1:A:433:ARG:CZ	2.99	0.41
1:A:87:LEU:HD23	1:A:430:ALA:O	2.21	0.41
1:A:230:HIS:HD2	4:B:501:PLM:HC1	1.86	0.41
1:B:205:PHE:CE1	1:B:300:GLU:HG2	2.56	0.41
1:A:264:ILE:HD11	1:A:291:VAL:HG21	2.01	0.41
1:A:270:LYS:O	1:A:274:GLU:HG2	2.20	0.41
1:A:381:ILE:HA	1:A:382:PRO:HD2	1.89	0.41
1:A:429:SER:O	1:A:434:ILE:HG13	2.21	0.41
1:B:182:VAL:O	1:B:264:ILE:HG12	2.20	0.41
1:B:447:LEU:HA	1:B:447:LEU:HD23	1.88	0.41
1:A:97:ARG:NH2	3:A:500:HEM:O2A	2.51	0.41
1:A:236:ASN:HD22	1:A:236:ASN:HA	1.56	0.41
1:B:30:PRO:HA	1:B:31:PRO:HD3	1.91	0.41
1:B:64:VAL:HG21	1:B:376:PHE:HE2	1.86	0.41
1:B:210:SER:HA	1:B:211:PRO:HD3	1.82	0.41
1:A:124:ARG:HE	1:A:128:LEU:HD11	1.86	0.40
1:A:160:LYS:O	1:A:161:ALA:HB3	2.21	0.40
1:B:80:TYR:HA	1:B:394:VAL:HG22	2.04	0.40
1:A:104:GLN:O	1:A:108:LYS:HA	2.22	0.40
1:B:375:LYS:NZ	1:B:380:LEU:CD1	2.84	0.40
1:A:323:VAL:HG11	1:A:453:LEU:HD12	2.02	0.40
1:B:99:ASN:HD22	1:B:100:SER:N	2.19	0.40
1:B:232:LYS:HD2	1:B:232:LYS:HA	1.85	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	461/476 (97%)	429 (93%)	23 (5%)	9 (2%)	6 16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	461/476 (97%)	408 (88%)	43 (9%)	10 (2%)	5	14
All	All	922/952 (97%)	837 (91%)	66 (7%)	19 (2%)	5	15

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	277	ASN
1	A	278	GLN
1	B	275	LYS
1	A	42	MET
1	A	189	TYR
1	A	279	LYS
1	A	377	ARG
1	B	48	LYS
1	B	278	GLN
1	B	279	LYS
1	B	377	ARG
1	A	415	LYS
1	A	48	LYS
1	A	462	ASP
1	B	189	TYR
1	B	404	PRO
1	B	461	VAL
1	B	227	PRO
1	B	106	ILE

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	419/430 (97%)	373 (89%)	46 (11%)	6	15
1	B	419/430 (97%)	376 (90%)	43 (10%)	7	18
All	All	838/860 (97%)	749 (89%)	89 (11%)	6	17

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	35	PRO
1	A	37	PRO
1	A	38	ILE
1	A	39	ILE
1	A	42	MET
1	A	43	LEU
1	A	50	ILE
1	A	51	CYS
1	A	97	ARG
1	A	99	ASN
1	A	100	SER
1	A	101	PRO
1	A	104	GLN
1	A	125	ARG
1	A	153	VAL
1	A	170	LEU
1	A	192	GLN
1	A	200	ARG
1	A	213	ILE
1	A	215	VAL
1	A	231	ASN
1	A	236	ASN
1	A	259	ASN
1	A	273	GLN
1	A	276	ASP
1	A	278	GLN
1	A	279	LYS
1	A	290	THR
1	A	307	ARG
1	A	314	LEU
1	A	322	LYS
1	A	325	GLU
1	A	335	ARG
1	A	372	THR
1	A	377	ARG
1	A	380	LEU
1	A	388	MET
1	A	398	ASP
1	A	413	LEU
1	A	415	LYS
1	A	465	LYS
1	A	466	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	472	VAL
1	A	476	ILE
1	A	482	SER
1	B	28	LYS
1	B	37	PRO
1	B	38	ILE
1	B	39	ILE
1	B	43	LEU
1	B	44	GLN
1	B	50	ILE
1	B	67	VAL
1	B	75	VAL
1	B	87	LEU
1	B	92	GLU
1	B	99	ASN
1	B	104	GLN
1	B	112	ILE
1	B	170	LEU
1	B	181	VAL
1	B	184	GLN
1	B	193	ASN
1	B	209	ASN
1	B	215	VAL
1	B	222	LEU
1	B	231	ASN
1	B	239	LEU
1	B	273	GLN
1	B	276	ASP
1	B	279	LYS
1	B	286	ASN
1	B	308	TYR
1	B	314	LEU
1	B	325	GLU
1	B	328	ASP
1	B	340	GLN
1	B	374	THR
1	B	377	ARG
1	B	388	MET
1	B	413	LEU
1	B	415	LYS
1	B	442	ARG
1	B	461	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	465	LYS
1	B	468	ASN
1	B	472	VAL
1	B	476	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	99	ASN
1	A	192	GLN
1	A	193	ASN
1	A	202	ASN
1	A	209	ASN
1	A	214	GLN
1	A	230	HIS
1	A	236	ASN
1	A	259	ASN
1	A	286	ASN
1	A	340	GLN
1	A	378	ASN
1	A	405	ASN
1	A	416	ASN
1	A	457	ASN
1	A	468	ASN
1	B	56	ASN
1	B	99	ASN
1	B	192	GLN
1	B	193	ASN
1	B	204	ASN
1	B	209	ASN
1	B	236	ASN
1	B	286	ASN
1	B	324	GLN
1	B	378	ASN
1	B	396	HIS
1	B	457	ASN
1	B	468	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

5 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	PLM	B	501	-	17,17,17	0.50	0	17,17,17	0.82	0
2	PO4	A	504	-	4,4,4	2.42	2 (50%)	6,6,6	0.88	0
3	HEM	B	500	1	50,50,50	2.38	25 (50%)	67,82,82	1.22	10 (14%)
4	PLM	A	502	-	17,17,17	0.52	0	17,17,17	0.94	0
3	HEM	A	500	1	50,50,50	2.46	24 (48%)	67,82,82	1.26	11 (16%)

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	B	500	1	-	6/14/54/54	-
4	PLM	A	502	-	-	2/15/15/15	-
4	PLM	B	501	-	-	1/15/15/15	-
3	HEM	A	500	1	-	4/14/54/54	-

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	HEM	C1D-ND	-5.14	1.28	1.38
3	A	500	HEM	C4A-NA	-4.96	1.30	1.39
3	B	500	HEM	C1D-ND	-4.43	1.30	1.38
3	A	500	HEM	C1B-NB	-4.31	1.32	1.40
3	A	500	HEM	FE-ND	4.22	2.07	1.94
3	B	500	HEM	C4B-NB	-4.20	1.30	1.38
2	A	504	PO4	P-O1	4.17	1.60	1.50
3	B	500	HEM	C4D-ND	-4.10	1.33	1.40
3	B	500	HEM	C4A-NA	-4.04	1.32	1.39
3	B	500	HEM	C1C-NC	-4.04	1.32	1.39
3	B	500	HEM	FE-ND	3.98	2.07	1.94
3	A	500	HEM	C4D-ND	-3.94	1.33	1.40
3	A	500	HEM	CAC-C3C	-3.90	1.37	1.47
3	B	500	HEM	CAC-C3C	-3.83	1.37	1.47
3	A	500	HEM	C1C-C2C	-3.83	1.37	1.45
3	A	500	HEM	CBB-CAB	3.78	1.48	1.30
3	B	500	HEM	CMA-C3A	3.64	1.58	1.50
3	B	500	HEM	C1B-NB	-3.55	1.34	1.40
3	A	500	HEM	C1C-NC	-3.53	1.33	1.39
3	B	500	HEM	FE-NA	3.48	2.06	1.95
3	B	500	HEM	CBB-CAB	3.42	1.46	1.30
3	B	500	HEM	C1C-C2C	-3.32	1.38	1.45
3	A	500	HEM	C1D-C2D	-3.27	1.37	1.44
3	A	500	HEM	C4B-NB	-3.22	1.32	1.38
3	B	500	HEM	FE-NB	3.22	2.04	1.94
3	A	500	HEM	C4D-C3D	-3.18	1.39	1.45
3	A	500	HEM	FE-NB	3.17	2.04	1.94
3	A	500	HEM	FE-NA	3.17	2.05	1.95
3	B	500	HEM	CAB-C3B	-2.89	1.39	1.47
3	A	500	HEM	C4C-NC	-2.81	1.34	1.39
3	B	500	HEM	CMC-C2C	2.80	1.56	1.50
3	B	500	HEM	FE-NC	2.59	2.03	1.95
3	A	500	HEM	CMA-C3A	2.49	1.55	1.50
3	A	500	HEM	FE-NC	2.49	2.03	1.95
3	B	500	HEM	O2A-CGA	-2.44	1.22	1.30
3	B	500	HEM	CBC-CAC	2.44	1.42	1.30
3	A	500	HEM	CBD-CGD	2.41	1.56	1.50
3	B	500	HEM	C4D-C3D	-2.39	1.41	1.45
3	A	500	HEM	CBC-CAC	2.35	1.41	1.30
3	A	500	HEM	C3B-C2B	2.34	1.41	1.37
3	A	500	HEM	C3C-C4C	-2.32	1.42	1.46
3	B	500	HEM	C1A-NA	-2.25	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	500	HEM	C3C-C4C	-2.25	1.42	1.46
3	B	500	HEM	CAD-C3D	2.23	1.57	1.51
3	A	500	HEM	CMC-C2C	2.22	1.55	1.50
2	A	504	PO4	P-O3	2.21	1.61	1.54
3	A	500	HEM	O2A-CGA	-2.20	1.23	1.30
3	B	500	HEM	C4C-NC	-2.16	1.35	1.39
3	B	500	HEM	C1D-C2D	-2.12	1.40	1.44
3	A	500	HEM	CAB-C3B	-2.07	1.41	1.47
3	B	500	HEM	CBD-CGD	2.02	1.55	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	HEM	C4C-C3C-C2C	-2.68	104.49	106.81
3	B	500	HEM	C1C-CHC-C4B	2.56	131.47	126.02
3	A	500	HEM	C3B-C4B-NB	2.50	111.26	109.47
3	A	500	HEM	CHD-C4C-NC	-2.45	121.78	124.45
3	B	500	HEM	CHD-C4C-NC	-2.40	121.84	124.45
3	A	500	HEM	C3B-C2B-C1B	-2.40	104.61	106.41
3	A	500	HEM	C1B-NB-C4B	2.39	108.04	105.21
3	A	500	HEM	C4B-C3B-C2B	-2.38	105.09	107.28
3	B	500	HEM	C3B-C2B-C1B	-2.35	104.64	106.41
3	A	500	HEM	C1C-CHC-C4B	2.30	130.91	126.02
3	A	500	HEM	O2A-CGA-CBA	2.29	121.24	114.00
3	B	500	HEM	C4C-C3C-C2C	-2.27	104.84	106.81
3	B	500	HEM	O2A-CGA-CBA	2.22	121.01	114.00
3	B	500	HEM	C1B-NB-C4B	2.20	107.81	105.21
3	A	500	HEM	C4D-ND-C1D	2.20	107.81	105.21
3	B	500	HEM	C4D-ND-C1D	2.15	107.75	105.21
3	A	500	HEM	C4A-CHB-C1B	2.15	131.29	126.25
3	B	500	HEM	C4B-C3B-C2B	-2.09	105.36	107.28
3	A	500	HEM	C4C-CHD-C1D	2.04	130.35	126.02
3	B	500	HEM	C4A-CHB-C1B	2.03	131.02	126.25
3	B	500	HEM	C3B-C4B-NB	2.02	110.92	109.47

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	502	PLM	CC-CD-CE-CF
4	B	501	PLM	C8-C9-CA-CB
3	A	500	HEM	C2C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

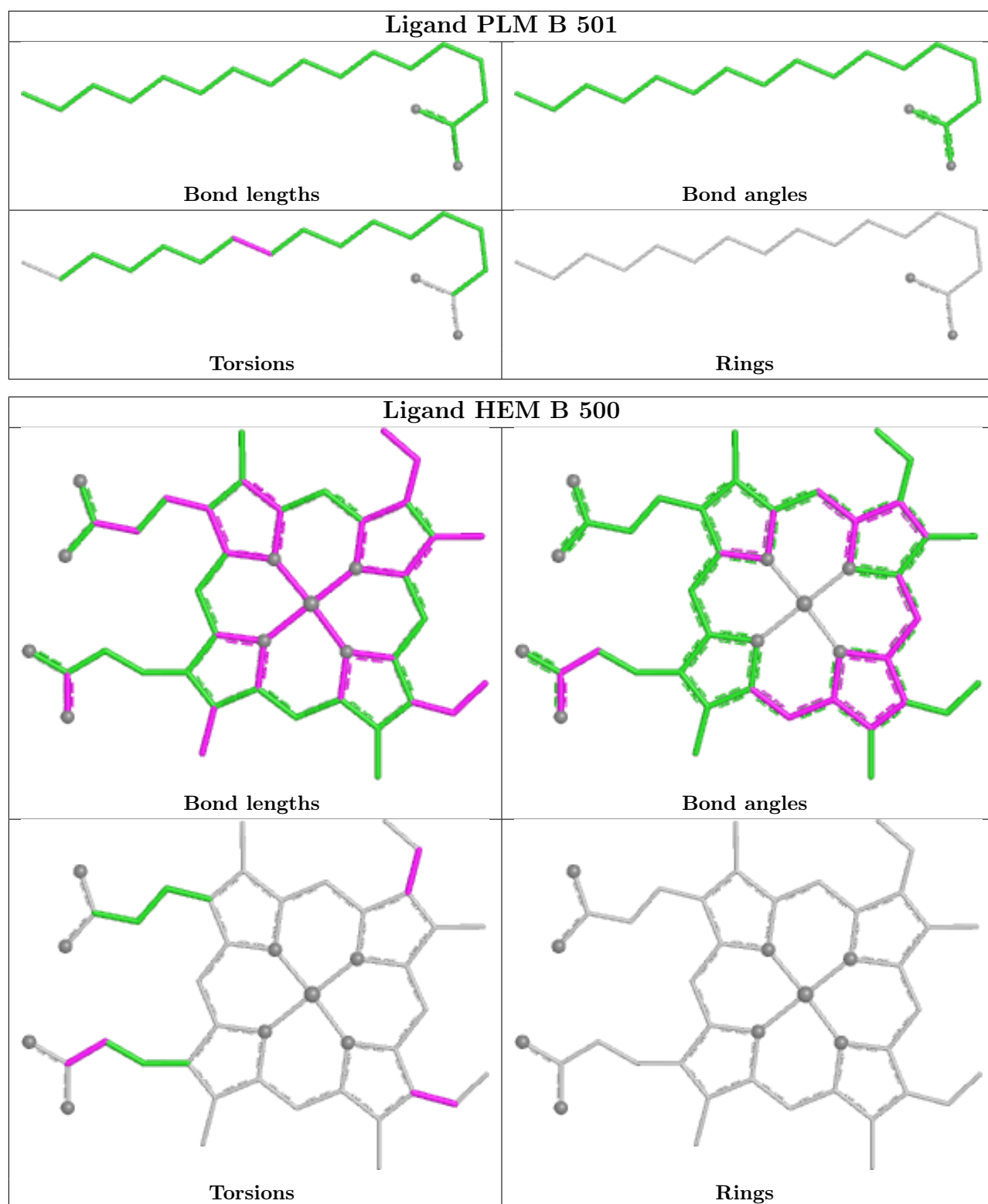
Mol	Chain	Res	Type	Atoms
3	B	500	HEM	C2C-C3C-CAC-CBC
3	B	500	HEM	C2B-C3B-CAB-CBB
3	A	500	HEM	C4C-C3C-CAC-CBC
3	B	500	HEM	C4B-C3B-CAB-CBB
3	B	500	HEM	C4C-C3C-CAC-CBC
3	B	500	HEM	CAA-CBA-CGA-O1A
3	A	500	HEM	CAA-CBA-CGA-O2A
3	A	500	HEM	CAA-CBA-CGA-O1A
3	B	500	HEM	CAA-CBA-CGA-O2A
4	A	502	PLM	O1-C1-C2-C3

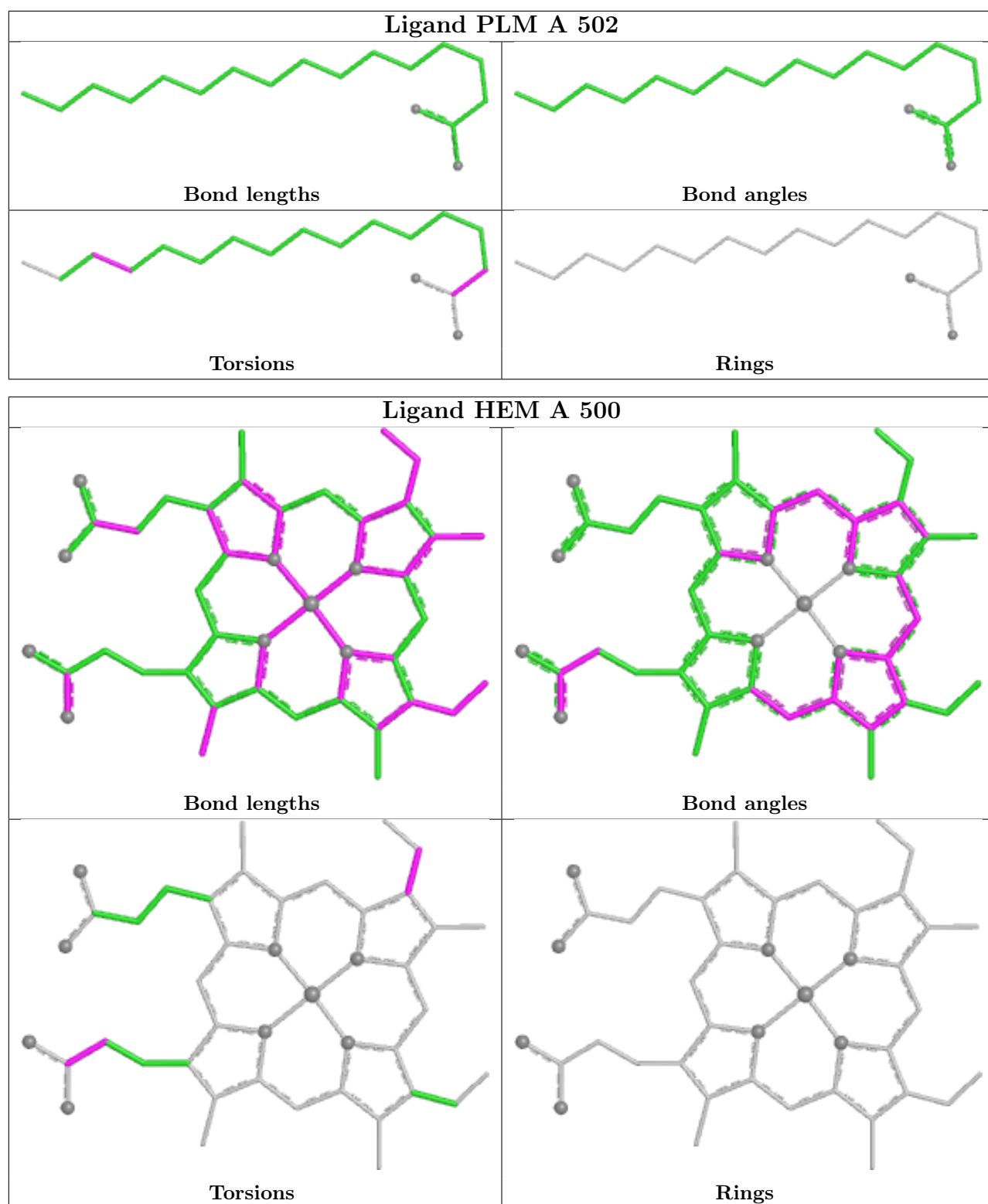
There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	PLM	6	0
3	B	500	HEM	2	0
4	A	502	PLM	3	0
3	A	500	HEM	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	463/476 (97%)	0.26	12 (2%) 57 54	28, 58, 84, 112	0
1	B	463/476 (97%)	0.41	17 (3%) 45 41	34, 65, 96, 109	0
All	All	926/952 (97%)	0.34	29 (3%) 51 48	28, 61, 92, 112	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	GLY	6.2
1	A	490	VAL	5.5
1	B	490	VAL	4.7
1	A	96	GLY	4.6
1	A	97	ARG	3.6
1	B	472	VAL	3.6
1	A	99	ASN	3.3
1	A	278	GLN	3.1
1	B	47	VAL	3.0
1	B	453	LEU	2.7
1	B	279	LYS	2.6
1	A	184	GLN	2.6
1	A	35	PRO	2.5
1	A	273	GLN	2.4
1	B	196	THR	2.4
1	B	150	HIS	2.3
1	A	277	ASN	2.3
1	B	489	PRO	2.3
1	B	331	ILE	2.3
1	B	473	THR	2.2
1	B	206	ARG	2.2
1	B	277	ASN	2.2
1	B	468	ASN	2.2
1	A	384	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	257	VAL	2.2
1	B	488	ILE	2.1
1	A	262	ASP	2.1
1	B	184	GLN	2.1
1	B	246	GLU	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](#)

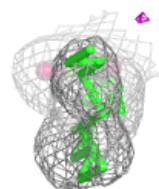
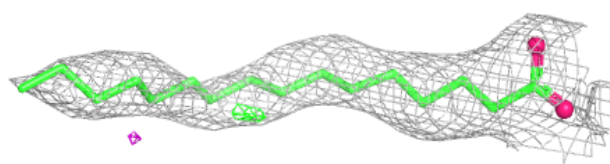
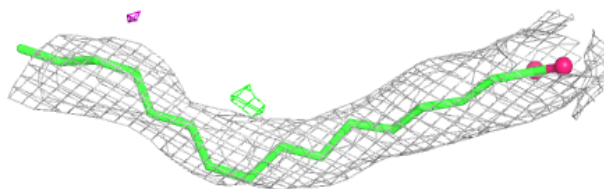
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PO4	A	504	5/5	0.85	0.12	91,92,93,93	0
4	PLM	A	502	18/18	0.86	0.15	53,58,70,72	0
4	PLM	B	501	18/18	0.89	0.12	56,59,62,64	0
3	HEM	A	500	43/43	0.97	0.08	37,42,49,53	0
3	HEM	B	500	43/43	0.97	0.08	39,44,45,49	0

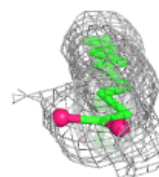
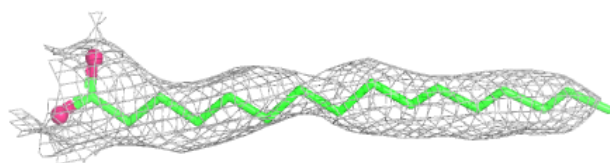
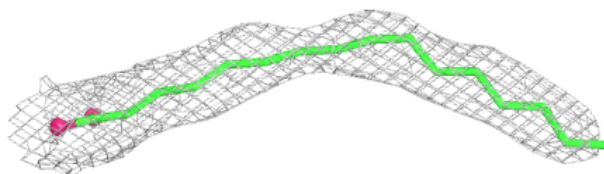
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PLM A 502:

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

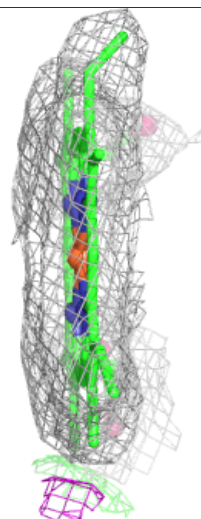
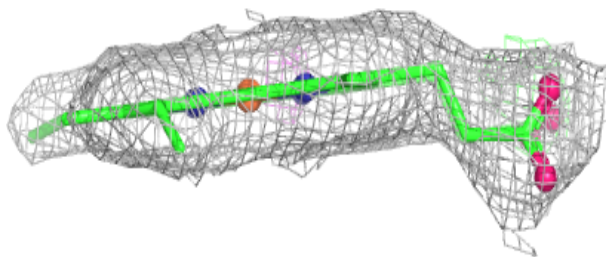
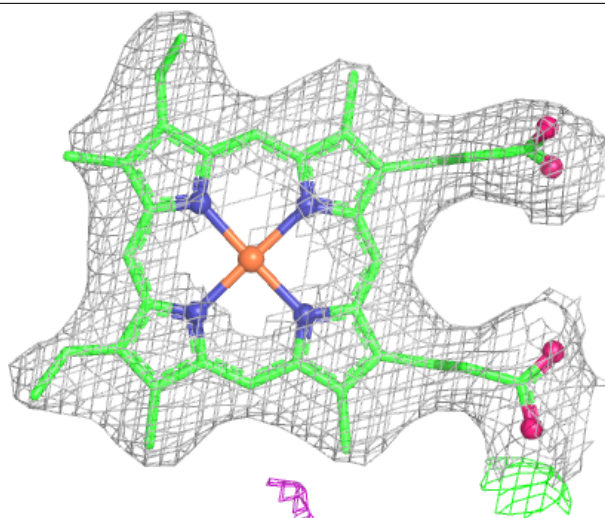
**Electron density around PLM B 501:**

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



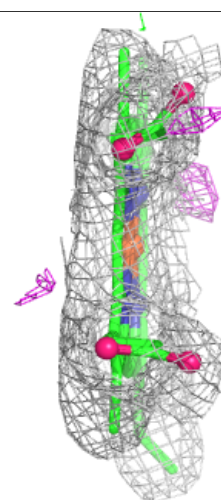
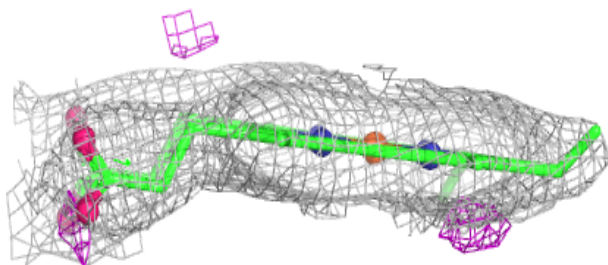
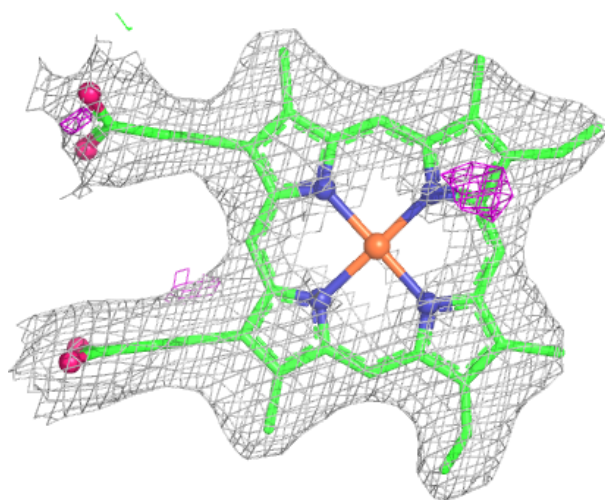
Electron density around HEM A 500:

$2mF_o-DF_c$ (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)



6.5 Other polymers ⓘ

There are no such residues in this entry.