



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 03:16 PM EDT

PDB ID : 3TDA / pdb_00003tda
Title : Competitive replacement of thioridazine by prinomastat in crystals of cytochrome P450 2D6
Authors : Wang, A.; Stout, C.D.; Johnson, E.F.
Deposited on : 2011-08-10
Resolution : 2.67 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

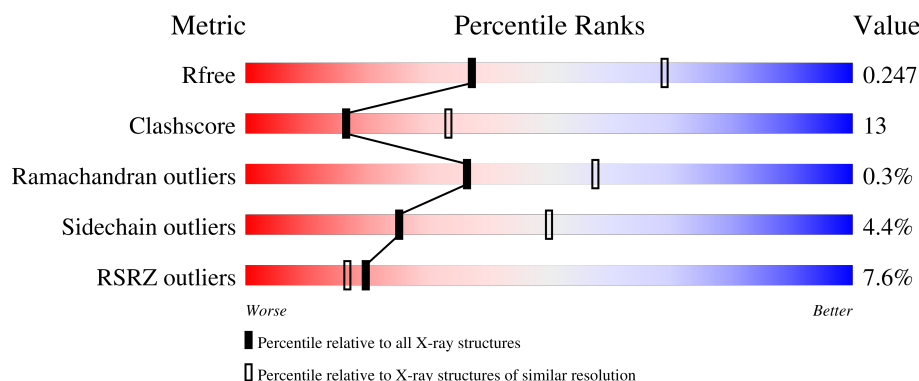
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	479	5% 72% 24% • •
1	B	479	8% 68% 25% • 5%
1	C	479	9% 71% 24% • •
1	D	479	8% 68% 25% • 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15106 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 2D6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	0	0
			3690	2367	654	655	14			
1	B	456	Total	C	N	O	S	0	0	0
			3614	2317	640	643	14			
1	C	467	Total	C	N	O	S	0	0	0
			3690	2367	654	655	14			
1	D	456	Total	C	N	O	S	0	0	0
			3614	2317	640	643	14			

There are 60 discrepancies between the modelled and reference sequences:

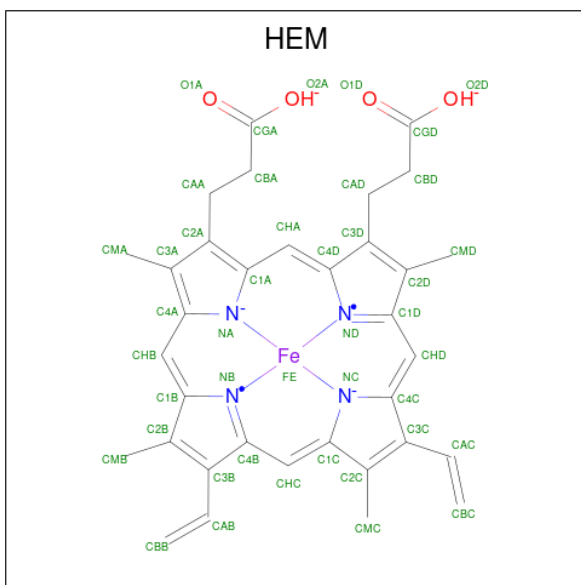
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	expression tag	UNP P10635
A	24	ALA	-	expression tag	UNP P10635
A	25	LYS	-	expression tag	UNP P10635
A	26	LYS	-	expression tag	UNP P10635
A	27	THR	-	expression tag	UNP P10635
A	28	SER	-	expression tag	UNP P10635
A	29	SER	-	expression tag	UNP P10635
A	30	LYS	-	expression tag	UNP P10635
A	31	GLY	-	expression tag	UNP P10635
A	32	LYS	-	expression tag	UNP P10635
A	33	LEU	-	expression tag	UNP P10635
A	498	HIS	-	expression tag	UNP P10635
A	499	HIS	-	expression tag	UNP P10635
A	500	HIS	-	expression tag	UNP P10635
A	501	HIS	-	expression tag	UNP P10635
B	23	MET	-	expression tag	UNP P10635
B	24	ALA	-	expression tag	UNP P10635
B	25	LYS	-	expression tag	UNP P10635
B	26	LYS	-	expression tag	UNP P10635
B	27	THR	-	expression tag	UNP P10635
B	28	SER	-	expression tag	UNP P10635

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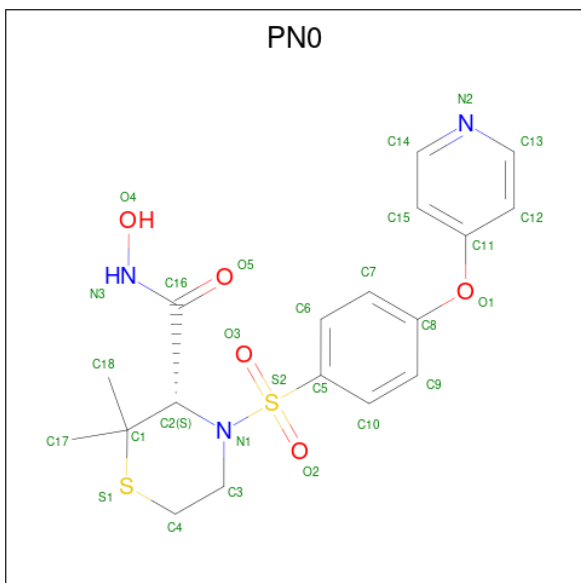
Chain	Residue	Modelled	Actual	Comment	Reference
B	29	SER	-	expression tag	UNP P10635
B	30	LYS	-	expression tag	UNP P10635
B	31	GLY	-	expression tag	UNP P10635
B	32	LYS	-	expression tag	UNP P10635
B	33	LEU	-	expression tag	UNP P10635
B	498	HIS	-	expression tag	UNP P10635
B	499	HIS	-	expression tag	UNP P10635
B	500	HIS	-	expression tag	UNP P10635
B	501	HIS	-	expression tag	UNP P10635
C	23	MET	-	expression tag	UNP P10635
C	24	ALA	-	expression tag	UNP P10635
C	25	LYS	-	expression tag	UNP P10635
C	26	LYS	-	expression tag	UNP P10635
C	27	THR	-	expression tag	UNP P10635
C	28	SER	-	expression tag	UNP P10635
C	29	SER	-	expression tag	UNP P10635
C	30	LYS	-	expression tag	UNP P10635
C	31	GLY	-	expression tag	UNP P10635
C	32	LYS	-	expression tag	UNP P10635
C	33	LEU	-	expression tag	UNP P10635
C	498	HIS	-	expression tag	UNP P10635
C	499	HIS	-	expression tag	UNP P10635
C	500	HIS	-	expression tag	UNP P10635
C	501	HIS	-	expression tag	UNP P10635
D	23	MET	-	expression tag	UNP P10635
D	24	ALA	-	expression tag	UNP P10635
D	25	LYS	-	expression tag	UNP P10635
D	26	LYS	-	expression tag	UNP P10635
D	27	THR	-	expression tag	UNP P10635
D	28	SER	-	expression tag	UNP P10635
D	29	SER	-	expression tag	UNP P10635
D	30	LYS	-	expression tag	UNP P10635
D	31	GLY	-	expression tag	UNP P10635
D	32	LYS	-	expression tag	UNP P10635
D	33	LEU	-	expression tag	UNP P10635
D	498	HIS	-	expression tag	UNP P10635
D	499	HIS	-	expression tag	UNP P10635
D	500	HIS	-	expression tag	UNP P10635
D	501	HIS	-	expression tag	UNP P10635

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



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

- Molecule 3 is Prinomastat (CCD ID: PN0) (formula: $C_{18}H_{21}N_3O_5S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			28	18	3	5	2		
3	B	1	Total	C	N	O	S	0	0
			28	18	3	5	2		
3	C	1	Total	C	N	O	S	0	0
			28	18	3	5	2		
3	D	1	Total	C	N	O	S	0	0
			28	18	3	5	2		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		
4	B	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		

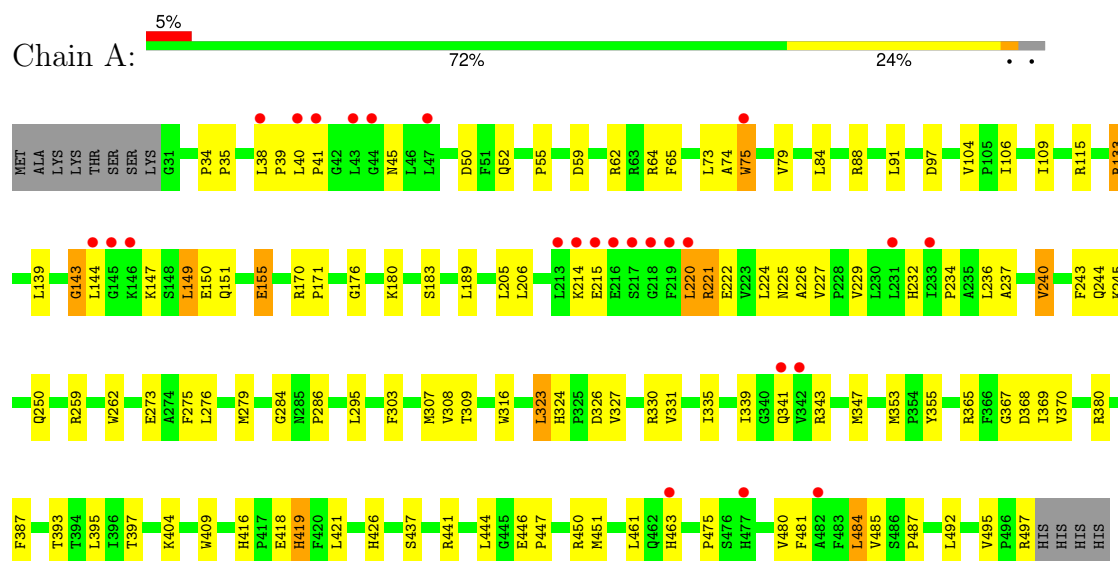
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	61	Total	O	0	0
			61	61		
5	B	48	Total	O	0	0
			48	48		
5	C	63	Total	O	0	0
			63	63		
5	D	37	Total	O	0	0
			37	37		

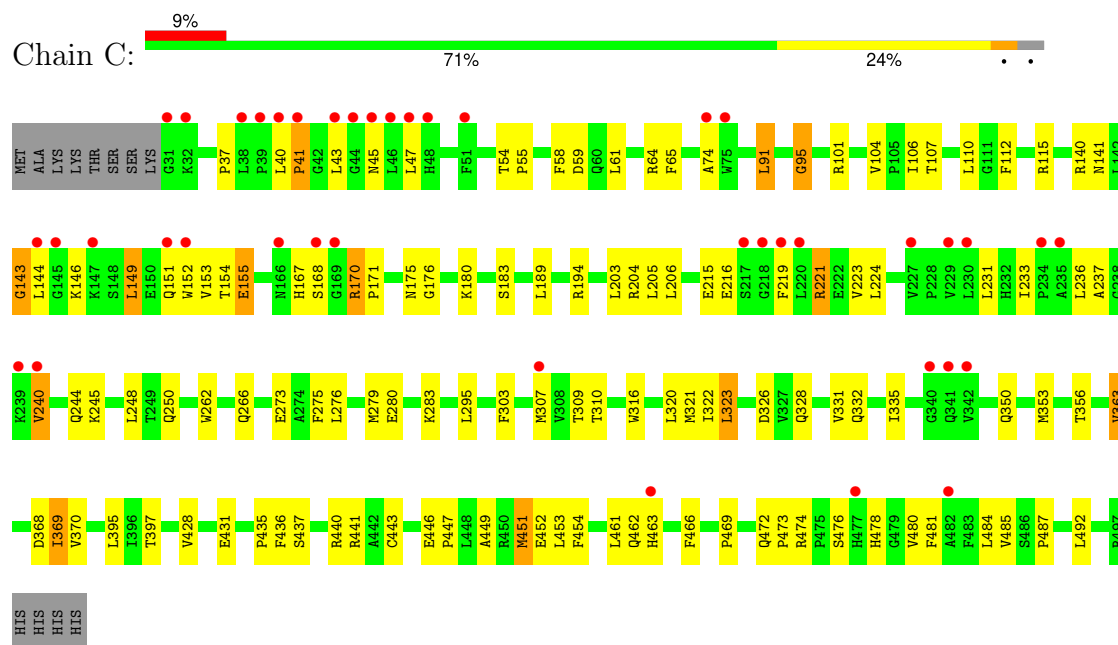
3 Residue-property plots [i](#)

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.

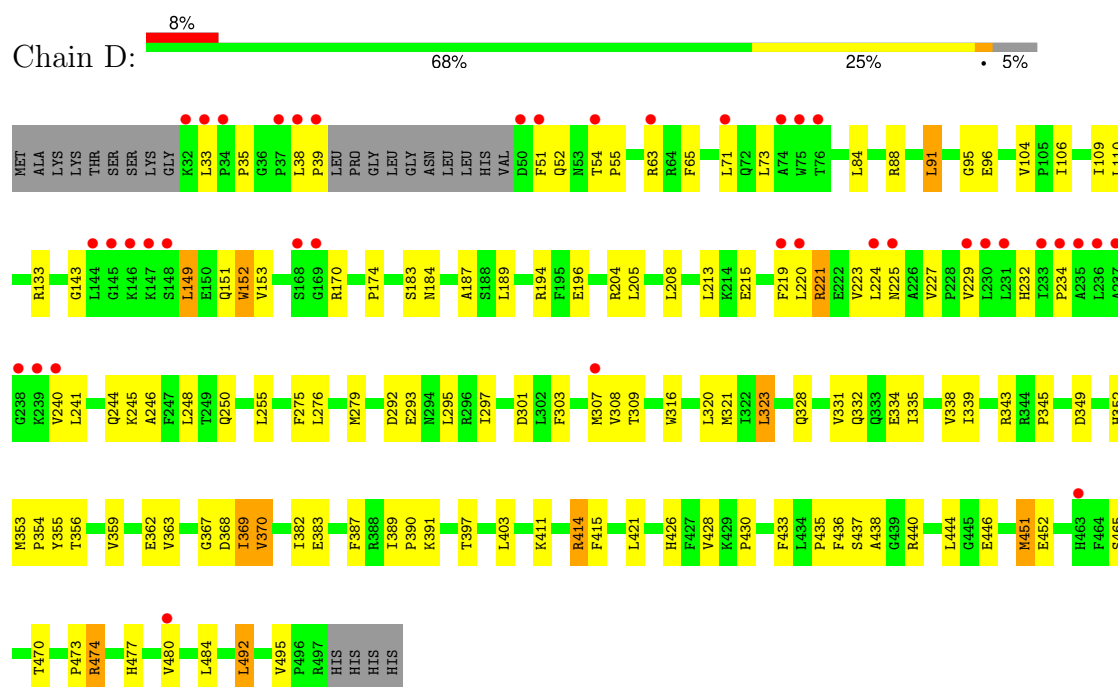
• Molecule 1: Cytochrome P450 2D6



• Molecule 1: Cytochrome P450 2D6



• Molecule 1: Cytochrome P450 2D6



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.05Å 192.74Å 247.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.04 – 2.67 42.04 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.04-2.67) 99.7 (42.04-2.67)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.18 (at 2.69Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.217 , 0.255 0.208 , 0.247	Depositor DCC
R_{free} test set	3916 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.3	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	0.94	EDS
Total number of atoms	15106	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.09 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.3835e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: ZN, PN0, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.57	0/3790	0.95	6/5155 (0.1%)
1	B	0.54	0/3711	0.97	11/5045 (0.2%)
1	C	0.57	0/3790	0.98	12/5155 (0.2%)
1	D	0.53	0/3711	0.96	9/5045 (0.2%)
All	All	0.55	0/15002	0.97	38/20400 (0.2%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	240	VAL	N-CA-C	7.81	117.92	110.42
1	D	51	PHE	N-CA-C	-6.62	103.88	112.23
1	B	411	LYS	CA-C-N	6.54	128.02	119.84
1	B	411	LYS	C-N-CA	6.54	128.02	119.84
1	C	168	SER	CB-CA-C	-6.08	108.56	115.79
1	C	170	ARG	N-CA-C	6.04	116.55	109.60
1	A	485	VAL	N-CA-C	5.95	117.01	107.73
1	C	155	GLU	N-CA-C	-5.75	104.93	111.14
1	C	91	LEU	CA-C-N	-5.70	117.39	122.97
1	C	91	LEU	C-N-CA	-5.70	117.39	122.97
1	A	155	GLU	N-CA-C	-5.61	105.08	111.14
1	C	91	LEU	N-CA-C	5.60	118.32	111.82
1	D	369	ILE	N-CA-C	5.57	118.02	111.05
1	B	307	MET	N-CA-C	5.48	117.33	111.36
1	C	95	GLY	N-CA-C	5.36	119.13	112.64
1	C	485	VAL	N-CA-C	5.35	116.46	108.54
1	A	419	HIS	N-CA-C	-5.35	105.62	111.82
1	D	292	ASP	N-CA-C	5.32	117.76	111.33
1	A	214	LYS	N-CA-C	-5.30	106.94	113.41
1	B	483	PHE	N-CA-C	-5.25	105.47	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	HIS	CA-C-N	5.24	125.29	119.32
1	A	324	HIS	C-N-CA	5.24	125.29	119.32
1	D	474	ARG	CA-C-N	5.19	125.17	120.03
1	D	474	ARG	C-N-CA	5.19	125.17	120.03
1	B	196	GLU	N-CA-C	-5.18	103.30	110.35
1	D	370	VAL	CA-C-N	5.18	126.31	119.84
1	D	370	VAL	C-N-CA	5.18	126.31	119.84
1	C	175	ASN	N-CA-C	5.15	117.31	111.02
1	C	74	ALA	CB-CA-C	-5.14	110.67	116.63
1	B	260	MET	N-CA-C	5.12	116.94	111.36
1	D	91	LEU	N-CA-C	5.11	118.67	112.23
1	B	324	HIS	CA-C-N	5.11	125.39	119.47
1	B	324	HIS	C-N-CA	5.11	125.39	119.47
1	C	363	VAL	N-CA-C	-5.07	105.76	110.53
1	D	338	VAL	CB-CA-C	-5.06	106.44	111.30
1	B	147	LYS	N-CA-C	5.04	117.51	111.71
1	B	344	ARG	CA-C-N	5.02	125.01	119.89
1	B	344	ARG	C-N-CA	5.02	125.01	119.89

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	3690	0	3679	87	0
1	B	3614	0	3596	90	0
1	C	3690	0	3679	97	0
1	D	3614	0	3596	105	0
2	A	43	0	30	4	0
2	B	43	0	30	2	0
2	C	43	0	30	6	0
2	D	43	0	30	3	0
3	A	28	0	21	3	0
3	B	28	0	21	0	0
3	C	28	0	21	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	28	0	21	1	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	61	0	0	4	0
5	B	48	0	0	2	0
5	C	63	0	0	2	0
5	D	37	0	0	0	0
All	All	15106	0	14754	381	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 13.

All (381) 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:32:LYS:NZ	1:B:32:LYS:HA	1.80	0.94
1:A:133:ARG:HH11	1:A:133:ARG:HA	1.36	0.90
1:D:279:MET:HE1	1:D:295:LEU:HD22	1.52	0.89
1:D:440:ARG:HH21	1:D:440:ARG:HG3	1.36	0.89
1:D:220:LEU:HB3	1:D:240:VAL:HG12	1.61	0.83
1:B:303:PHE:CD1	1:B:307:MET:CE	2.63	0.82
1:A:40:LEU:HB3	1:A:41:PRO:HD2	1.63	0.81
1:A:369:ILE:HG13	1:A:370:VAL:HG23	1.63	0.78
1:B:38:LEU:HD12	1:B:39:PRO:HD2	1.66	0.78
1:C:206:LEU:HD23	1:C:307:MET:HE2	1.67	0.76
1:B:32:LYS:HA	1:B:32:LYS:HZ2	1.48	0.76
1:C:221:ARG:HH11	1:C:221:ARG:HG2	1.52	0.75
1:B:143:GLY:O	1:B:146:LYS:HG2	1.88	0.74
1:B:32:LYS:HA	1:B:32:LYS:HZ3	1.50	0.73
1:C:369:ILE:HG13	1:C:370:VAL:HG23	1.70	0.73
1:B:440:ARG:HG3	1:B:440:ARG:HH21	1.51	0.73
1:C:55:PRO:HD3	1:C:481:PHE:CE1	2.24	0.72
1:D:440:ARG:HG3	1:D:440:ARG:NH2	2.04	0.72
1:D:369:ILE:HG13	1:D:370:VAL:HG23	1.69	0.72
1:A:183:SER:OG	1:A:307:MET:HB2	1.90	0.71
1:D:309:THR:HB	2:D:800:HEM:HAB	1.73	0.71
1:C:55:PRO:CG	1:C:481:PHE:CE1	2.74	0.70
1:C:224:LEU:HD22	1:C:240:VAL:HG11	1.72	0.70
1:A:224:LEU:HD21	1:A:236:LEU:HD13	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:LEU:HD22	1:D:248:LEU:HD12	1.74	0.69
1:D:54:THR:HB	1:D:55:PRO:HD3	1.74	0.69
1:A:38:LEU:HD12	1:A:39:PRO:HD2	1.73	0.69
1:A:279:MET:HE1	1:A:295:LEU:HD22	1.74	0.69
1:D:35:PRO:HD3	1:D:387:PHE:CE1	2.28	0.69
1:A:262:TRP:CD1	1:A:273:GLU:HG2	2.27	0.68
1:C:40:LEU:HG	1:C:41:PRO:HD2	1.76	0.68
1:B:303:PHE:CD1	1:B:307:MET:HE1	2.29	0.68
1:C:219:PHE:O	1:C:223:VAL:HG23	1.94	0.67
1:C:143:GLY:O	1:C:146:LYS:HB2	1.95	0.67
1:D:414:ARG:HG3	1:D:414:ARG:HH11	1.59	0.66
1:A:59:ASP:HA	1:A:62:ARG:NH1	2.10	0.66
1:B:279:MET:HE1	1:B:295:LEU:HD22	1.77	0.66
1:D:328:GLN:O	1:D:332:GLN:HG3	1.95	0.66
1:A:55:PRO:HD3	1:A:481:PHE:CE1	2.30	0.65
1:B:451:MET:HG3	1:B:452:GLU:N	2.09	0.65
1:B:54:THR:N	1:B:55:PRO:HD2	2.12	0.65
1:D:38:LEU:HB2	1:D:39:PRO:HD3	1.79	0.65
1:B:143:GLY:HA2	1:B:146:LYS:HE3	1.80	0.64
1:C:55:PRO:HD3	1:C:481:PHE:CZ	2.32	0.64
1:D:321:MET:HE2	1:D:321:MET:HA	1.78	0.64
1:C:55:PRO:CD	1:C:481:PHE:CE1	2.80	0.64
1:B:104:VAL:HG12	1:B:107:THR:HG23	1.79	0.64
1:B:85:ALA:HB3	5:B:522:HOH:O	1.98	0.64
1:B:309:THR:HB	2:B:800:HEM:HAB	1.80	0.63
1:A:206:LEU:HD23	1:A:307:MET:SD	2.39	0.63
1:A:232:HIS:O	1:A:234:PRO:HD3	1.99	0.63
1:B:474:ARG:HG2	1:B:474:ARG:HH11	1.63	0.63
1:B:227:VAL:HG12	1:B:229:VAL:HG12	1.80	0.62
1:D:149:LEU:O	1:D:153:VAL:HG23	2.00	0.62
1:A:59:ASP:HA	1:A:62:ARG:HH12	1.65	0.62
1:A:303:PHE:CD1	1:A:307:MET:CE	2.83	0.62
1:C:224:LEU:HD23	1:C:231:LEU:HD23	1.81	0.61
1:D:303:PHE:CE2	1:D:307:MET:HE2	2.35	0.61
1:C:368:ASP:HB3	5:C:530:HOH:O	2.00	0.61
1:D:63:ARG:HG2	1:D:63:ARG:HH11	1.64	0.61
1:B:440:ARG:HG3	1:B:440:ARG:NH2	2.15	0.61
1:A:446:GLU:HB3	1:A:447:PRO:HD3	1.82	0.61
1:D:414:ARG:HH11	1:D:414:ARG:CG	2.14	0.60
1:D:303:PHE:HE2	1:D:307:MET:HE2	1.66	0.60
1:C:276:LEU:HD23	1:C:279:MET:HE3	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:GLU:HA	1:C:221:ARG:NH1	2.17	0.59
1:B:220:LEU:HD13	1:B:224:LEU:HD13	1.83	0.59
1:B:233:ILE:HB	1:B:236:LEU:HD23	1.85	0.59
1:D:275:PHE:CD2	1:D:295:LEU:HD13	2.37	0.59
1:A:91:LEU:HD11	1:A:397:THR:HG21	1.84	0.59
1:A:276:LEU:HA	1:A:279:MET:HE3	1.83	0.59
1:D:359:VAL:O	1:D:363:VAL:HG23	2.01	0.59
1:C:279:MET:HE1	1:C:295:LEU:HD22	1.85	0.59
1:B:226:ALA:O	1:B:228:PRO:HD3	2.02	0.58
1:A:221:ARG:O	1:A:225:ASN:HB2	2.04	0.58
1:B:105:PRO:O	1:B:108:GLN:HG3	2.02	0.58
1:D:63:ARG:HG2	1:D:63:ARG:NH1	2.17	0.58
1:D:104:VAL:HA	1:D:225:ASN:HD21	1.69	0.58
1:C:233:ILE:N	1:C:233:ILE:HD12	2.19	0.58
1:C:328:GLN:O	1:C:332:GLN:HG3	2.03	0.58
1:D:205:LEU:HD13	1:D:250:GLN:HG3	1.86	0.57
1:A:276:LEU:HD23	1:A:279:MET:HE3	1.85	0.57
1:A:50:ASP:OD1	1:A:52:GLN:HG2	2.04	0.57
1:D:221:ARG:O	1:D:225:ASN:HB2	2.04	0.57
1:A:276:LEU:HD23	1:A:279:MET:CE	2.34	0.57
1:D:213:LEU:HD22	1:D:308:VAL:HG21	1.86	0.57
1:A:335:ILE:HG12	1:A:353:MET:HE1	1.85	0.57
1:C:309:THR:HB	2:C:800:HEM:HAB	1.87	0.57
1:D:276:LEU:HD23	1:D:279:MET:HE3	1.87	0.57
1:A:109:ILE:CG2	1:A:245:LYS:HD2	2.35	0.57
1:D:352:HIS:C	1:D:354:PRO:HD3	2.29	0.57
1:C:276:LEU:HD23	1:C:279:MET:CE	2.36	0.56
1:D:219:PHE:O	1:D:223:VAL:HG23	2.05	0.56
1:D:227:VAL:HG12	1:D:229:VAL:HG12	1.87	0.56
1:A:339:ILE:HG23	1:A:343:ARG:NH1	2.20	0.56
1:B:303:PHE:HD1	1:B:307:MET:CE	2.18	0.56
1:C:233:ILE:HD12	1:C:233:ILE:H	1.71	0.56
1:D:331:VAL:HG13	1:D:356:THR:OG1	2.06	0.56
1:A:75:TRP:CZ3	1:A:226:ALA:HB2	2.41	0.55
1:D:95:GLY:HA3	1:D:440:ARG:NH2	2.21	0.55
1:D:33:LEU:HD12	1:D:33:LEU:N	2.21	0.55
1:B:105:PRO:HD2	1:B:225:ASN:OD1	2.06	0.55
1:D:152:TRP:HH2	1:D:194:ARG:HB3	1.71	0.55
1:D:183:SER:OG	1:D:307:MET:HB2	2.07	0.55
1:C:110:LEU:HD22	1:C:248:LEU:HD12	1.88	0.54
1:B:139:LEU:HB3	1:B:144:LEU:HD12	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:HIS:CE1	1:D:426:HIS:HE2	2.25	0.54
1:B:91:LEU:HD11	1:B:397:THR:HG21	1.89	0.54
1:B:224:LEU:HD21	1:B:236:LEU:HB3	1.90	0.54
1:D:208:LEU:HD22	1:D:246:ALA:HB3	1.88	0.54
1:D:382:ILE:HG13	1:D:389:ILE:HB	1.89	0.54
1:D:35:PRO:HB2	1:D:65:PHE:HB3	1.90	0.54
1:B:334:GLU:OE1	1:B:353:MET:HA	2.07	0.54
1:A:84:LEU:O	1:A:88:ARG:HB2	2.07	0.53
1:A:308:VAL:HG22	1:A:308:VAL:O	2.08	0.53
1:D:339:ILE:HG12	1:D:349:ASP:OD1	2.07	0.53
1:B:474:ARG:HG2	1:B:474:ARG:NH1	2.21	0.53
1:B:89:GLU:O	1:B:93:THR:HB	2.08	0.53
1:C:245:LYS:NZ	1:C:245:LYS:HB3	2.23	0.53
1:A:104:VAL:HG12	1:A:106:ILE:HG22	1.91	0.53
1:D:196:GLU:OE1	1:D:196:GLU:HA	2.08	0.53
1:C:40:LEU:HD23	1:C:43:LEU:HD12	1.90	0.53
1:B:174:PRO:HD3	1:B:492:LEU:HD22	1.91	0.53
1:D:335:ILE:HG12	1:D:353:MET:HE1	1.89	0.53
1:D:109:ILE:HG22	1:D:245:LYS:HE2	1.91	0.52
1:D:215:GLU:O	1:D:221:ARG:HG2	2.09	0.52
1:A:97:ASP:OD2	1:A:380:ARG:HD2	2.09	0.52
1:A:275:PHE:HD2	1:A:279:MET:HE2	1.74	0.52
1:D:84:LEU:HD11	1:D:88:ARG:HD2	1.91	0.52
1:D:170:ARG:HG3	1:D:170:ARG:HH11	1.75	0.52
1:B:355:TYR:O	1:B:359:VAL:HG23	2.09	0.52
1:B:104:VAL:CG1	1:B:107:THR:HG23	2.40	0.52
1:B:303:PHE:CE1	1:B:307:MET:CE	2.92	0.52
1:D:91:LEU:HD11	1:D:397:THR:HG21	1.91	0.52
1:C:215:GLU:OE1	1:C:244:GLN:HG3	2.10	0.52
1:A:151:GLN:O	1:A:155:GLU:HG3	2.10	0.52
1:D:232:HIS:O	1:D:234:PRO:HD3	2.09	0.52
1:B:331:VAL:HG13	1:B:356:THR:OG1	2.10	0.51
1:C:303:PHE:CE1	1:C:307:MET:HE3	2.46	0.51
1:B:104:VAL:HA	1:B:225:ASN:HD21	1.75	0.51
1:C:183:SER:OG	1:C:307:MET:HG3	2.10	0.51
1:D:71:LEU:HD12	1:D:71:LEU:O	2.10	0.51
1:D:38:LEU:N	1:D:38:LEU:HD12	2.25	0.51
1:C:476:SER:C	1:C:478:HIS:H	2.17	0.51
1:B:60:GLN:O	1:B:64:ARG:HG3	2.11	0.51
1:B:105:PRO:HD2	1:B:225:ASN:CG	2.35	0.51
1:A:441:ARG:HB2	5:A:530:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:800:HEM:C1D	3:A:503:PN0:H14	2.45	0.51
1:B:59:ASP:O	1:B:63:ARG:HD3	2.11	0.50
1:C:335:ILE:HG12	1:C:353:MET:HE1	1.92	0.50
1:A:450:ARG:HD2	5:A:550:HOH:O	2.12	0.50
1:D:71:LEU:CD1	1:D:73:LEU:HG	2.41	0.50
1:C:473:PRO:O	1:C:474:ARG:C	2.53	0.50
1:D:215:GLU:OE1	1:D:244:GLN:HG3	2.12	0.50
1:B:319:LEU:HB2	1:B:490:TYR:CE2	2.47	0.50
1:C:321:MET:HE2	1:C:321:MET:HA	1.94	0.50
1:A:369:ILE:HD12	1:A:484:LEU:HD11	1.94	0.50
1:D:428:VAL:O	1:D:430:PRO:HD3	2.12	0.50
1:C:469:PRO:HB2	1:C:472:GLN:NE2	2.27	0.50
1:D:334:GLU:OE1	1:D:353:MET:HA	2.12	0.50
1:B:220:LEU:HD13	1:B:220:LEU:C	2.37	0.49
1:B:377:MET:HA	1:B:393:THR:O	2.12	0.49
1:B:424:GLN:HB2	1:B:426:HIS:CE1	2.47	0.49
1:C:104:VAL:HG12	1:C:106:ILE:HG22	1.94	0.49
1:C:152:TRP:HH2	1:C:194:ARG:HB3	1.76	0.49
1:B:445:GLY:HA3	2:B:800:HEM:C3C	2.47	0.49
1:A:104:VAL:HA	1:A:225:ASN:HD21	1.78	0.49
1:A:215:GLU:OE1	1:A:243:PHE:HB2	2.13	0.49
1:D:369:ILE:HG13	1:D:370:VAL:CG2	2.41	0.49
1:C:350:GLN:HG3	1:C:454:PHE:CD2	2.48	0.49
1:C:221:ARG:HH11	1:C:221:ARG:CG	2.22	0.49
1:C:262:TRP:CD1	1:C:273:GLU:HG2	2.48	0.49
1:D:106:ILE:HD11	1:D:240:VAL:HG21	1.95	0.49
1:C:326:ASP:OD2	1:C:326:ASP:N	2.46	0.49
2:D:800:HEM:C1D	3:D:503:PN0:H14	2.48	0.49
1:B:132:ARG:HD2	1:B:444:LEU:HD12	1.94	0.48
1:B:422:ASP:OD1	1:B:424:GLN:HG3	2.13	0.48
1:D:339:ILE:HA	1:D:343:ARG:HH12	1.79	0.48
1:A:88:ARG:CZ	5:A:512:HOH:O	2.61	0.48
1:A:409:TRP:O	1:D:411:LYS:NZ	2.45	0.48
1:C:276:LEU:HA	1:C:279:MET:HE3	1.95	0.48
1:D:421:LEU:HA	1:D:426:HIS:O	2.13	0.48
1:B:336:ASP:CG	1:B:497:ARG:HH22	2.21	0.48
1:B:420:PHE:O	1:B:427:PHE:HA	2.14	0.48
1:B:129:ARG:NH1	5:B:512:HOH:O	2.47	0.48
1:D:38:LEU:HD12	1:D:38:LEU:H	1.77	0.48
1:B:303:PHE:O	1:B:307:MET:HE3	2.13	0.48
1:D:309:THR:HB	2:D:800:HEM:CAB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:ARG:HA	1:C:144:LEU:HB2	1.96	0.48
1:C:101:ARG:HG2	1:C:441:ARG:NH2	2.29	0.48
1:A:40:LEU:HB3	1:A:41:PRO:CD	2.39	0.47
1:D:106:ILE:HG13	1:D:241:LEU:HD11	1.96	0.47
1:B:336:ASP:OD2	1:B:497:ARG:NH2	2.47	0.47
1:C:440:ARG:HH21	1:C:440:ARG:HG3	1.79	0.47
1:D:275:PHE:CD2	1:D:279:MET:HE2	2.48	0.47
1:A:224:LEU:HD12	1:A:240:VAL:HG11	1.97	0.47
2:A:800:HEM:ND	3:A:503:PN0:H14	2.29	0.47
1:B:266:GLN:HG3	1:B:267:PRO:HD2	1.96	0.47
1:C:43:LEU:HD13	1:C:47:LEU:HD11	1.97	0.47
1:C:91:LEU:HD11	1:C:397:THR:HG21	1.95	0.47
1:D:451:MET:HG3	1:D:452:GLU:N	2.30	0.47
1:C:205:LEU:HD13	1:C:250:GLN:HG3	1.95	0.47
1:A:40:LEU:CB	1:A:41:PRO:HD2	2.37	0.47
1:A:149:LEU:HB3	1:A:451:MET:HE1	1.96	0.47
1:C:152:TRP:CE3	1:C:152:TRP:O	2.67	0.47
1:C:206:LEU:CD2	1:C:307:MET:HE2	2.41	0.47
1:C:322:ILE:HG22	1:C:466:PHE:C	2.40	0.47
1:A:205:LEU:HD13	1:A:250:GLN:CG	2.45	0.47
1:B:54:THR:HG21	1:B:372:LEU:HD11	1.97	0.47
1:C:205:LEU:HD13	1:C:250:GLN:CG	2.45	0.47
1:D:414:ARG:CG	1:D:414:ARG:NH1	2.74	0.47
1:C:280:GLU:OE2	1:C:283:LYS:HE2	2.15	0.47
1:D:308:VAL:HG22	1:D:308:VAL:O	2.15	0.47
1:D:293:GLU:OE1	1:D:293:GLU:N	2.45	0.47
1:C:180:LYS:HE2	1:C:203:LEU:CD2	2.45	0.46
1:D:187:ALA:HB2	1:D:303:PHE:HE1	1.80	0.46
1:D:339:ILE:HD13	1:D:345:PRO:HB3	1.97	0.46
1:B:220:LEU:O	1:B:224:LEU:HD13	2.15	0.46
1:A:170:ARG:HA	1:A:171:PRO:HD3	1.84	0.46
1:A:341:GLN:HE22	1:A:497:ARG:C	2.23	0.46
1:B:307:MET:HE3	1:B:307:MET:HB2	1.77	0.46
1:C:435:PRO:HG2	1:C:436:PHE:CD1	2.50	0.46
1:D:382:ILE:CG1	1:D:389:ILE:HB	2.45	0.46
1:B:176:GLY:O	1:B:180:LYS:HG3	2.16	0.46
1:C:443:CYS:HB2	2:C:800:HEM:NA	2.29	0.46
1:C:152:TRP:CH2	1:C:194:ARG:HB3	2.50	0.46
1:C:446:GLU:HB3	1:C:447:PRO:HD3	1.97	0.46
1:D:383:GLU:HA	1:D:387:PHE:O	2.16	0.46
1:D:316:TRP:O	1:D:320:LEU:HG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:440:ARG:NH2	1:D:440:ARG:CG	2.72	0.46
1:A:64:ARG:HD2	1:A:65:PHE:CZ	2.51	0.46
1:C:176:GLY:O	1:C:180:LYS:HG3	2.15	0.46
1:A:330:ARG:HB2	1:A:355:TYR:CE2	2.51	0.45
1:C:216:GLU:HA	1:C:221:ARG:HH12	1.81	0.45
1:D:205:LEU:HD13	1:D:250:GLN:CG	2.47	0.45
1:D:436:PHE:CE1	1:D:446:GLU:HG3	2.51	0.45
1:A:35:PRO:HD3	1:A:387:PHE:CE2	2.52	0.45
1:A:437:SER:HB3	2:A:800:HEM:HBA1	1.99	0.45
1:D:275:PHE:HD2	1:D:279:MET:HE2	1.82	0.45
1:D:174:PRO:HD3	1:D:492:LEU:HD22	1.98	0.45
1:D:444:LEU:C	1:D:444:LEU:HD12	2.41	0.45
1:A:88:ARG:HG2	1:A:88:ARG:HH11	1.81	0.45
1:A:227:VAL:HG12	1:A:229:VAL:HG22	1.99	0.45
1:C:275:PHE:HD2	1:C:279:MET:HE2	1.81	0.45
1:C:449:ALA:O	1:C:453:LEU:HG	2.16	0.45
1:D:367:GLY:O	1:D:368:ASP:C	2.59	0.45
1:B:144:LEU:HD21	1:B:448:LEU:HA	1.98	0.45
1:B:380:ARG:HG2	1:B:381:ASP:N	2.32	0.45
1:C:151:GLN:O	1:C:155:GLU:HG3	2.17	0.45
1:D:110:LEU:HD22	1:D:248:LEU:CD1	2.44	0.45
1:D:480:VAL:HG13	1:D:480:VAL:O	2.16	0.45
1:A:416:HIS:HB3	1:A:419:HIS:CE1	2.51	0.45
1:B:183:SER:OG	1:B:307:MET:HG3	2.17	0.45
1:A:284:GLY:O	1:A:286:PRO:HD3	2.16	0.45
1:A:327:VAL:O	1:A:331:VAL:HG23	2.17	0.45
1:C:323:LEU:HD12	1:C:323:LEU:HA	1.87	0.45
1:C:331:VAL:HG11	1:C:461:LEU:HD12	1.99	0.45
1:B:54:THR:N	1:B:55:PRO:CD	2.80	0.44
1:D:184:ASN:ND2	1:D:194:ARG:HB2	2.32	0.44
1:A:79:VAL:HG23	1:A:393:THR:HG21	1.99	0.44
1:A:176:GLY:O	1:A:180:LYS:HG3	2.16	0.44
1:C:151:GLN:HA	1:C:154:THR:OG1	2.18	0.44
1:A:244:GLN:HG2	3:A:503:PN0:H4	1.98	0.44
1:C:55:PRO:HG2	1:C:481:PHE:CE1	2.53	0.44
1:D:473:PRO:O	1:D:474:ARG:C	2.59	0.44
1:A:416:HIS:NE2	1:A:418:GLU:HB2	2.31	0.44
1:D:303:PHE:HE2	1:D:307:MET:CE	2.29	0.44
1:C:180:LYS:HG2	1:C:206:LEU:CD1	2.46	0.44
1:C:451:MET:HG3	1:C:452:GLU:N	2.33	0.44
1:A:303:PHE:CE1	1:A:307:MET:CE	3.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:LEU:O	1:C:153:VAL:HG23	2.18	0.44
1:B:199:ASP:O	1:B:203:LEU:HG	2.17	0.44
1:B:303:PHE:CE1	1:B:307:MET:HE2	2.53	0.44
1:C:180:LYS:HG2	1:C:206:LEU:HD11	2.00	0.44
1:C:233:ILE:H	1:C:233:ILE:CD1	2.30	0.44
1:D:133:ARG:HA	1:D:133:ARG:HD3	1.88	0.44
1:D:362:GLU:HG3	1:D:415:PHE:CD1	2.53	0.44
1:C:43:LEU:CD1	1:C:47:LEU:HD11	2.48	0.44
1:A:303:PHE:CE1	1:A:307:MET:HE2	2.52	0.44
1:A:444:LEU:C	1:A:444:LEU:HD12	2.43	0.44
1:B:106:ILE:C	1:B:108:GLN:H	2.25	0.44
1:C:37:PRO:HG2	1:C:45:ASN:ND2	2.32	0.44
1:B:469:PRO:HB2	1:B:472:GLN:CD	2.43	0.43
1:A:150:GLU:HG2	1:A:347:MET:HG2	2.00	0.43
1:A:275:PHE:CD2	1:A:279:MET:HE2	2.53	0.43
1:B:106:ILE:C	1:B:108:GLN:N	2.76	0.43
1:C:54:THR:N	1:C:55:PRO:CD	2.81	0.43
1:A:369:ILE:HG13	1:A:370:VAL:CG2	2.43	0.43
1:C:320:LEU:HD12	1:C:363:VAL:HG22	2.01	0.43
1:A:109:ILE:O	1:A:109:ILE:HG22	2.17	0.43
1:A:221:ARG:HG3	1:A:222:GLU:N	2.33	0.43
1:A:421:LEU:HA	1:A:426:HIS:O	2.19	0.43
1:B:226:ALA:C	1:B:228:PRO:HD3	2.44	0.43
1:B:490:TYR:CD1	1:B:490:TYR:C	2.96	0.43
1:A:88:ARG:NE	5:A:512:HOH:O	2.51	0.43
1:B:220:LEU:HD13	1:B:220:LEU:O	2.18	0.43
1:D:153:VAL:HG21	1:D:451:MET:SD	2.59	0.43
1:D:433:PHE:CZ	1:D:435:PRO:HG3	2.53	0.43
1:A:73:LEU:O	1:A:74:ALA:HB3	2.19	0.43
1:C:309:THR:HB	2:C:800:HEM:CAB	2.47	0.43
1:B:219:PHE:O	1:B:223:VAL:HG23	2.19	0.43
1:B:328:GLN:O	1:B:332:GLN:HG3	2.18	0.43
1:A:39:PRO:HA	1:A:45:ASN:ND2	2.34	0.43
1:A:323:LEU:CD1	1:A:475:PRO:HD2	2.49	0.43
1:B:144:LEU:HA	1:B:149:LEU:HD12	2.01	0.43
1:C:441:ARG:HD2	2:C:800:HEM:O2D	2.18	0.43
1:C:104:VAL:CG1	1:C:106:ILE:HG22	2.49	0.42
1:C:141:ASN:O	1:C:146:LYS:HE2	2.19	0.42
1:B:70:SER:O	1:B:71:LEU:HD23	2.19	0.42
1:D:323:LEU:HD12	1:D:323:LEU:HA	1.89	0.42
1:A:139:LEU:HB3	1:A:144:LEU:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ASP:N	1:A:326:ASP:OD2	2.51	0.42
1:C:40:LEU:HG	1:C:41:PRO:CD	2.47	0.42
1:C:221:ARG:NH1	1:C:221:ARG:CG	2.83	0.42
1:D:104:VAL:HG12	1:D:225:ASN:HD21	1.85	0.42
1:A:237:ALA:HA	1:A:240:VAL:CG2	2.50	0.42
1:B:323:LEU:HD13	1:B:475:PRO:HG2	2.01	0.42
1:D:276:LEU:HD23	1:D:279:MET:CE	2.49	0.42
1:C:40:LEU:HD22	1:C:47:LEU:HD12	2.01	0.42
1:D:170:ARG:HG3	1:D:170:ARG:NH1	2.33	0.42
1:D:437:SER:OG	1:D:438:ALA:N	2.49	0.42
1:B:205:LEU:HD13	1:B:250:GLN:HB3	2.01	0.42
1:C:55:PRO:HG2	1:C:481:PHE:CD1	2.54	0.42
1:C:167:HIS:O	1:C:170:ARG:HB2	2.20	0.42
1:A:205:LEU:HD13	1:A:250:GLN:HG3	2.02	0.42
1:B:227:VAL:CG1	1:B:229:VAL:HG12	2.48	0.42
1:C:331:VAL:HG13	1:C:356:THR:OG1	2.20	0.42
1:A:331:VAL:HG11	1:A:461:LEU:HD12	2.02	0.42
1:C:64:ARG:HB3	1:C:65:PHE:CD1	2.55	0.42
1:C:170:ARG:HA	1:C:171:PRO:HD3	1.75	0.42
1:D:33:LEU:N	1:D:33:LEU:CD1	2.83	0.42
1:A:303:PHE:CD1	1:A:307:MET:HE2	2.53	0.41
1:B:192:GLY:O	1:B:269:ARG:NH2	2.53	0.41
1:C:437:SER:HB3	2:C:800:HEM:HBA1	2.02	0.41
1:D:71:LEU:HD12	1:D:71:LEU:C	2.45	0.41
1:B:321:MET:HE2	1:B:321:MET:HA	2.02	0.41
1:B:339:ILE:HG12	1:B:349:ASP:OD1	2.21	0.41
1:D:52:GLN:O	1:D:55:PRO:HD2	2.19	0.41
1:D:224:LEU:HD12	1:D:240:VAL:HG11	2.02	0.41
1:B:117:GLN:HB3	1:B:122:ALA:HA	2.03	0.41
1:B:320:LEU:HD13	1:B:415:PHE:CD1	2.55	0.41
2:C:800:HEM:C1D	3:C:503:PN0:H14	2.54	0.41
1:D:204:ARG:O	1:D:208:LEU:HG	2.20	0.41
1:D:321:MET:HA	1:D:321:MET:CE	2.50	0.41
1:D:355:TYR:O	1:D:359:VAL:HG23	2.20	0.41
1:D:428:VAL:O	1:D:428:VAL:HG23	2.20	0.41
1:A:367:GLY:O	1:A:368:ASP:C	2.64	0.41
1:C:58:PHE:HA	1:C:61:LEU:HD12	2.02	0.41
1:C:107:THR:HB	1:C:112:PHE:CD2	2.54	0.41
1:C:236:LEU:O	1:C:237:ALA:C	2.63	0.41
1:A:143:GLY:O	1:A:144:LEU:C	2.62	0.41
1:B:334:GLU:OE1	1:B:354:PRO:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:390:PRO:O	1:D:391:LYS:C	2.64	0.41
1:A:309:THR:HB	2:A:800:HEM:CAB	2.50	0.41
1:C:224:LEU:HD12	1:C:224:LEU:N	2.35	0.41
1:C:428:VAL:O	1:C:428:VAL:HG23	2.19	0.41
1:C:462:GLN:O	1:C:462:GLN:HG2	2.20	0.41
1:B:428:VAL:HG23	1:B:428:VAL:O	2.20	0.41
1:C:316:TRP:CD1	1:C:487:PRO:HD3	2.56	0.41
1:C:221:ARG:HG2	1:C:221:ARG:NH1	2.28	0.41
1:A:55:PRO:CD	1:A:481:PHE:CE1	3.01	0.41
1:A:220:LEU:CD2	1:A:224:LEU:HG	2.51	0.41
1:B:331:VAL:O	1:B:335:ILE:HG13	2.20	0.41
1:C:476:SER:C	1:C:478:HIS:N	2.79	0.41
1:B:275:PHE:HD2	1:B:279:MET:HE3	1.86	0.41
1:B:308:VAL:O	1:B:484:LEU:HD21	2.20	0.41
1:C:95:GLY:HA3	5:C:511:HOH:O	2.20	0.41
1:A:365:ARG:HH22	1:A:404:LYS:HD3	1.86	0.40
1:A:416:HIS:HB3	1:A:419:HIS:ND1	2.36	0.40
1:A:495:VAL:O	1:A:495:VAL:HG23	2.19	0.40
1:B:369:ILE:HG13	1:B:370:VAL:HG23	2.03	0.40
1:B:369:ILE:HG13	1:B:370:VAL:CG2	2.51	0.40
1:B:369:ILE:C	1:B:371:PRO:HD3	2.46	0.40
1:C:40:LEU:CD2	1:C:47:LEU:HD12	2.51	0.40
1:D:297:ILE:O	1:D:301:ASP:HB2	2.21	0.40
1:A:34:PRO:HA	1:A:387:PHE:CD2	2.56	0.40
1:A:316:TRP:CD1	1:A:487:PRO:HD3	2.56	0.40
1:B:84:LEU:HD11	1:B:88:ARG:HD2	2.03	0.40
1:D:495:VAL:O	1:D:495:VAL:HG23	2.21	0.40
1:D:321:MET:HE2	1:D:321:MET:CA	2.48	0.40
1:D:368:ASP:OD1	1:D:403:LEU:HD12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	465/479 (97%)	438 (94%)	26 (6%)	1 (0%)	43	65
1	B	452/479 (94%)	427 (94%)	24 (5%)	1 (0%)	43	65
1	C	465/479 (97%)	439 (94%)	24 (5%)	2 (0%)	30	51
1	D	452/479 (94%)	432 (96%)	19 (4%)	1 (0%)	43	65
All	All	1834/1916 (96%)	1736 (95%)	93 (5%)	5 (0%)	36	57

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	143	GLY
1	D	143	GLY
1	C	143	GLY
1	C	41	PRO
1	A	143	GLY

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	398/409 (97%)	382 (96%)	16 (4%)	28	53
1	B	390/409 (95%)	369 (95%)	21 (5%)	20	42
1	C	398/409 (97%)	381 (96%)	17 (4%)	26	51
1	D	390/409 (95%)	375 (96%)	15 (4%)	29	55
All	All	1576/1636 (96%)	1507 (96%)	69 (4%)	25	50

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	TRP
1	A	115	ARG
1	A	133	ARG
1	A	147	LYS
1	A	149	LEU
1	A	189	LEU

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Mol	Chain	Res	Type
1	A	220	LEU
1	A	221	ARG
1	A	240	VAL
1	A	259	ARG
1	A	323	LEU
1	A	395	LEU
1	A	463	HIS
1	A	480	VAL
1	A	484	LEU
1	A	492	LEU
1	B	32	LYS
1	B	52	GLN
1	B	75	TRP
1	B	149	LEU
1	B	154	THR
1	B	206	LEU
1	B	216	GLU
1	B	221	ARG
1	B	222	GLU
1	B	250	GLN
1	B	323	LEU
1	B	350	GLN
1	B	370	VAL
1	B	410	GLU
1	B	424	GLN
1	B	434	LEU
1	B	451	MET
1	B	465	SER
1	B	468	VAL
1	B	477	HIS
1	B	492	LEU
1	C	59	ASP
1	C	115	ARG
1	C	149	LEU
1	C	189	LEU
1	C	204	ARG
1	C	221	ARG
1	C	266	GLN
1	C	310	THR
1	C	323	LEU
1	C	369	ILE
1	C	395	LEU

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Mol	Chain	Res	Type
1	C	431	GLU
1	C	451	MET
1	C	463	HIS
1	C	480	VAL
1	C	484	LEU
1	C	492	LEU
1	D	96	GLU
1	D	149	LEU
1	D	151	GLN
1	D	152	TRP
1	D	189	LEU
1	D	221	ARG
1	D	255	LEU
1	D	323	LEU
1	D	414	ARG
1	D	451	MET
1	D	465	SER
1	D	470	THR
1	D	477	HIS
1	D	484	LEU
1	D	492	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	151	GLN
1	A	225	ASN
1	A	341	GLN
1	A	463	HIS
1	A	478	HIS
1	B	60	GLN
1	B	332	GLN
1	C	48	HIS
1	C	108	GLN
1	C	167	HIS
1	C	463	HIS
1	C	472	GLN
1	C	478	HIS
1	D	52	GLN
1	D	352	HIS
1	D	478	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	C	800	1,3	50,50,50	2.32	22 (44%)	67,82,82	1.29	10 (14%)
3	PN0	C	503	2	28,30,30	1.91	9 (32%)	37,44,44	1.80	8 (21%)
3	PN0	B	503	2	28,30,30	1.79	8 (28%)	37,44,44	1.81	7 (18%)
2	HEM	B	800	1,3	50,50,50	2.37	23 (46%)	67,82,82	1.33	11 (16%)
2	HEM	A	800	1,3	50,50,50	2.25	24 (48%)	67,82,82	1.29	9 (13%)
2	HEM	D	800	1,3	50,50,50	2.34	23 (46%)	67,82,82	1.36	11 (16%)
3	PN0	D	503	2	28,30,30	1.72	7 (25%)	37,44,44	1.83	7 (18%)
3	PN0	A	503	2	28,30,30	1.83	8 (28%)	37,44,44	1.80	7 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	C	800	1,3	-	6/14/54/54	-
3	PN0	C	503	2	-	6/21/39/39	0/3/3/3
3	PN0	B	503	2	-	8/21/39/39	0/3/3/3
2	HEM	B	800	1,3	-	7/14/54/54	-
2	HEM	A	800	1,3	-	5/14/54/54	-
2	HEM	D	800	1,3	-	7/14/54/54	-
3	PN0	D	503	2	-	6/21/39/39	0/3/3/3
3	PN0	A	503	2	-	8/21/39/39	0/3/3/3

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	503	PN0	C1-S1	-5.30	1.79	1.84
3	A	503	PN0	C1-S1	-5.02	1.79	1.84
2	B	800	HEM	C4D-ND	-4.72	1.32	1.40
2	A	800	HEM	FE-ND	4.61	2.09	1.94
2	B	800	HEM	C4A-NA	-4.42	1.31	1.39
2	D	800	HEM	C4D-ND	-4.42	1.32	1.40
2	B	800	HEM	FE-ND	4.37	2.08	1.94
2	B	800	HEM	C1D-ND	-4.27	1.30	1.38
2	C	800	HEM	C1D-ND	-4.22	1.30	1.38
2	C	800	HEM	FE-ND	4.22	2.07	1.94
2	D	800	HEM	C4A-NA	-4.19	1.31	1.39
2	D	800	HEM	C1D-ND	-4.18	1.30	1.38
2	C	800	HEM	C1B-NB	-4.13	1.33	1.40
2	C	800	HEM	CMA-C3A	4.11	1.59	1.50
2	A	800	HEM	C4D-ND	-4.01	1.33	1.40
2	C	800	HEM	C4D-ND	-3.98	1.33	1.40
2	D	800	HEM	FE-ND	3.96	2.07	1.94
2	B	800	HEM	C1B-NB	-3.94	1.33	1.40
2	C	800	HEM	C4A-NA	-3.90	1.32	1.39
2	A	800	HEM	C1D-ND	-3.85	1.31	1.38
2	A	800	HEM	C4A-NA	-3.85	1.32	1.39
3	B	503	PN0	C1-S1	-3.84	1.81	1.84
2	A	800	HEM	C1B-NB	-3.74	1.33	1.40
2	B	800	HEM	CMA-C3A	3.70	1.58	1.50
3	C	503	PN0	C15-C11	3.68	1.45	1.38
2	D	800	HEM	C1B-NB	-3.65	1.33	1.40
3	B	503	PN0	C5-S2	-3.64	1.71	1.76
2	A	800	HEM	CMA-C3A	3.61	1.58	1.50
2	B	800	HEM	C1C-NC	-3.55	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	800	HEM	CMA-C3A	3.52	1.58	1.50
2	B	800	HEM	FE-NB	3.51	2.05	1.94
2	A	800	HEM	CBB-CAB	3.50	1.47	1.30
2	C	800	HEM	FE-NB	3.50	2.05	1.94
2	B	800	HEM	CBB-CAB	3.50	1.47	1.30
3	D	503	PN0	C5-S2	-3.45	1.71	1.76
2	D	800	HEM	FE-NB	3.43	2.05	1.94
2	D	800	HEM	C1C-NC	-3.41	1.33	1.39
2	C	800	HEM	C1C-NC	-3.41	1.33	1.39
2	D	800	HEM	CBB-CAB	3.41	1.46	1.30
2	C	800	HEM	FE-NA	3.40	2.06	1.95
2	D	800	HEM	FE-NA	3.36	2.06	1.95
2	B	800	HEM	C4B-NB	-3.35	1.32	1.38
2	D	800	HEM	CAC-C3C	-3.31	1.38	1.47
2	B	800	HEM	C1C-C2C	-3.31	1.38	1.45
2	D	800	HEM	C1C-C2C	-3.28	1.38	1.45
3	D	503	PN0	C15-C11	3.28	1.44	1.38
2	C	800	HEM	FE-NC	3.27	2.06	1.95
2	A	800	HEM	FE-NA	3.27	2.06	1.95
2	D	800	HEM	FE-NC	3.25	2.05	1.95
2	C	800	HEM	CBB-CAB	3.24	1.46	1.30
2	A	800	HEM	FE-NC	3.22	2.05	1.95
2	B	800	HEM	CAC-C3C	-3.21	1.38	1.47
2	A	800	HEM	CAC-C3C	-3.21	1.38	1.47
3	D	503	PN0	C6-C5	3.21	1.43	1.38
3	B	503	PN0	C15-C11	3.15	1.44	1.38
2	B	800	HEM	FE-NA	3.12	2.05	1.95
2	A	800	HEM	C1C-NC	-3.11	1.33	1.39
2	C	800	HEM	C4B-NB	-3.09	1.32	1.38
3	A	503	PN0	C5-S2	-3.08	1.72	1.76
2	D	800	HEM	CMC-C2C	3.07	1.57	1.50
2	C	800	HEM	CMC-C2C	3.07	1.57	1.50
2	A	800	HEM	FE-NB	3.05	2.04	1.94
2	A	800	HEM	CMC-C2C	3.04	1.57	1.50
3	A	503	PN0	C15-C11	3.02	1.44	1.38
2	A	800	HEM	C4B-NB	-3.01	1.32	1.38
2	B	800	HEM	C3B-C2B	3.00	1.43	1.37
2	D	800	HEM	C4B-NB	-2.98	1.33	1.38
2	C	800	HEM	C3B-C2B	2.98	1.43	1.37
2	B	800	HEM	FE-NC	2.96	2.04	1.95
2	D	800	HEM	C3B-C2B	2.94	1.43	1.37
2	D	800	HEM	C4D-C3D	-2.92	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	503	PN0	C10-C5	2.90	1.43	1.38
2	C	800	HEM	C4D-C3D	-2.88	1.40	1.45
2	C	800	HEM	CAC-C3C	-2.84	1.39	1.47
3	A	503	PN0	C6-C5	2.79	1.43	1.38
3	C	503	PN0	C6-C5	2.71	1.43	1.38
2	B	800	HEM	CMC-C2C	2.70	1.56	1.50
3	C	503	PN0	C7-C8	2.70	1.43	1.38
3	A	503	PN0	C10-C5	2.69	1.43	1.38
2	D	800	HEM	O2A-CGA	-2.64	1.22	1.30
2	B	800	HEM	C4D-C3D	-2.61	1.40	1.45
3	B	503	PN0	C6-C5	2.58	1.42	1.38
2	D	800	HEM	CMD-C2D	2.56	1.56	1.50
2	C	800	HEM	C1C-C2C	-2.56	1.40	1.45
3	D	503	PN0	C1-S1	-2.56	1.82	1.84
2	A	800	HEM	C3B-C2B	2.50	1.42	1.37
2	D	800	HEM	C1D-C2D	-2.50	1.39	1.44
3	B	503	PN0	O3-S2	2.43	1.46	1.43
2	A	800	HEM	CMD-C2D	2.41	1.55	1.50
3	B	503	PN0	C7-C8	2.38	1.43	1.38
2	A	800	HEM	O2D-CGD	-2.38	1.22	1.30
2	A	800	HEM	O2A-CGA	-2.37	1.23	1.30
2	A	800	HEM	C1C-C2C	-2.36	1.40	1.45
3	C	503	PN0	C5-S2	-2.35	1.73	1.76
2	C	800	HEM	CBC-CAC	2.35	1.41	1.30
3	C	503	PN0	O3-S2	2.35	1.46	1.43
3	A	503	PN0	C7-C8	2.31	1.43	1.38
2	C	800	HEM	O2A-CGA	-2.30	1.23	1.30
3	A	503	PN0	O1-C11	-2.28	1.34	1.39
2	B	800	HEM	O2A-CGA	-2.28	1.23	1.30
3	A	503	PN0	O3-S2	2.28	1.45	1.43
3	D	503	PN0	C10-C5	2.28	1.42	1.38
2	A	800	HEM	C4D-C3D	-2.27	1.41	1.45
2	B	800	HEM	O2D-CGD	-2.26	1.23	1.30
3	C	503	PN0	O1-C11	-2.25	1.34	1.39
2	B	800	HEM	CBC-CAC	2.24	1.41	1.30
3	D	503	PN0	C7-C8	2.24	1.42	1.38
2	D	800	HEM	CBC-CAC	2.24	1.41	1.30
3	C	503	PN0	C9-C8	2.23	1.42	1.38
2	A	800	HEM	CAB-C3B	-2.23	1.41	1.47
2	D	800	HEM	C3C-C4C	-2.23	1.42	1.46
2	A	800	HEM	C3C-C4C	-2.21	1.42	1.46
3	B	503	PN0	O1-C11	-2.21	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	PN0	C15-C14	2.19	1.42	1.38
2	B	800	HEM	C4C-NC	-2.18	1.35	1.39
2	B	800	HEM	C1D-C2D	-2.17	1.40	1.44
3	D	503	PN0	O3-S2	2.17	1.45	1.43
2	B	800	HEM	C3C-C4C	-2.14	1.42	1.46
2	D	800	HEM	C3C-C2C	2.13	1.41	1.37
2	C	800	HEM	O2D-CGD	-2.12	1.23	1.30
2	C	800	HEM	CMD-C2D	2.12	1.55	1.50
2	A	800	HEM	CBC-CAC	2.09	1.40	1.30
2	A	800	HEM	C1D-C2D	-2.06	1.40	1.44
2	C	800	HEM	C4C-NC	-2.02	1.35	1.39

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	PN0	C18-C1-C17	-5.49	103.26	109.64
3	A	503	PN0	C18-C1-C17	-4.95	103.90	109.64
3	D	503	PN0	C11-O1-C8	4.93	130.04	118.78
3	C	503	PN0	C18-C1-C17	-4.84	104.02	109.64
3	D	503	PN0	C18-C1-C17	-4.83	104.03	109.64
3	C	503	PN0	O2-S2-C5	-4.79	102.14	108.10
3	D	503	PN0	O2-S2-C5	-4.68	102.28	108.10
3	A	503	PN0	O2-S2-C5	-4.53	102.48	108.10
3	B	503	PN0	O2-S2-C5	-4.41	102.62	108.10
3	C	503	PN0	C11-O1-C8	4.40	128.84	118.78
3	B	503	PN0	C11-O1-C8	4.33	128.68	118.78
3	A	503	PN0	C11-O1-C8	4.15	128.27	118.78
3	A	503	PN0	C5-S2-N1	3.94	114.23	107.36
2	D	800	HEM	CHD-C4C-NC	-3.54	120.60	124.45
3	B	503	PN0	C5-S2-N1	3.02	112.63	107.36
2	B	800	HEM	CHD-C4C-NC	-2.99	121.19	124.45
2	A	800	HEM	C3B-C4B-NB	2.97	111.60	109.47
2	D	800	HEM	CHC-C4B-NB	-2.90	121.31	124.42
3	C	503	PN0	C5-S2-N1	2.88	112.38	107.36
2	A	800	HEM	C4B-C3B-C2B	-2.86	104.65	107.28
2	D	800	HEM	C1B-NB-C4B	2.84	108.57	105.21
2	B	800	HEM	C4B-C3B-C2B	-2.82	104.68	107.28
3	D	503	PN0	O1-C11-C15	2.82	129.19	119.36
3	C	503	PN0	O1-C11-C15	2.80	129.09	119.36
2	D	800	HEM	C4B-C3B-C2B	-2.77	104.73	107.28
2	A	800	HEM	C1C-CHC-C4B	2.77	131.91	126.02
2	B	800	HEM	C3B-C4B-NB	2.76	111.45	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	PN0	O1-C11-C15	2.72	128.85	119.36
2	C	800	HEM	CHD-C4C-NC	-2.71	121.51	124.45
3	D	503	PN0	C3-N1-C2	2.70	123.41	116.20
3	A	503	PN0	O1-C11-C15	2.68	128.71	119.36
2	D	800	HEM	CHB-C1B-NB	-2.66	121.08	124.37
2	C	800	HEM	C4B-C3B-C2B	-2.65	104.85	107.28
3	D	503	PN0	O1-C11-C12	-2.60	110.31	119.36
3	C	503	PN0	C3-N1-C2	2.60	123.14	116.20
2	C	800	HEM	C1B-NB-C4B	2.58	108.26	105.21
3	C	503	PN0	O1-C11-C12	-2.57	110.42	119.36
2	C	800	HEM	C3B-C4B-NB	2.57	111.31	109.47
2	C	800	HEM	C1C-CHC-C4B	2.56	131.47	126.02
2	B	800	HEM	C1C-CHC-C4B	2.54	131.41	126.02
2	B	800	HEM	C1B-NB-C4B	2.53	108.20	105.21
2	B	800	HEM	CHC-C1C-NC	-2.51	121.72	124.45
3	B	503	PN0	C3-N1-C2	2.49	122.85	116.20
3	B	503	PN0	O1-C11-C12	-2.48	110.70	119.36
3	A	503	PN0	O1-C11-C12	-2.47	110.77	119.36
2	B	800	HEM	C4C-C3C-C2C	-2.46	104.68	106.81
2	A	800	HEM	CHC-C1C-NC	-2.43	121.80	124.45
3	A	503	PN0	C3-N1-C2	2.42	122.66	116.20
2	C	800	HEM	C3B-C2B-C1B	-2.39	104.61	106.41
2	D	800	HEM	C4D-ND-C1D	2.38	108.02	105.21
2	A	800	HEM	CHD-C4C-NC	-2.36	121.88	124.45
2	B	800	HEM	C3B-C2B-C1B	-2.33	104.66	106.41
2	C	800	HEM	C4D-ND-C1D	2.31	107.94	105.21
2	B	800	HEM	C4A-CHB-C1B	2.25	131.54	126.25
2	A	800	HEM	CHB-C1B-NB	-2.24	121.60	124.37
2	D	800	HEM	C3B-C4B-NB	2.22	111.06	109.47
2	D	800	HEM	CHC-C1C-NC	-2.19	122.07	124.45
2	B	800	HEM	CHB-C1B-NB	-2.19	121.66	124.37
3	D	503	PN0	C6-C5-S2	-2.18	117.57	119.73
2	C	800	HEM	CHB-C1B-NB	-2.17	121.69	124.37
2	A	800	HEM	C1B-NB-C4B	2.16	107.77	105.21
2	D	800	HEM	O2A-CGA-CBA	2.14	120.75	114.00
2	C	800	HEM	C4C-C3C-C2C	-2.13	104.96	106.81
2	C	800	HEM	C4A-CHB-C1B	2.11	131.21	126.25
2	D	800	HEM	C1C-CHC-C4B	2.09	130.46	126.02
2	A	800	HEM	C4D-ND-C1D	2.07	107.65	105.21
2	A	800	HEM	C4A-CHB-C1B	2.03	131.02	126.25
3	C	503	PN0	C3-C4-S1	2.02	114.81	112.47
2	B	800	HEM	C4D-ND-C1D	2.00	107.58	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	800	HEM	C3B-C2B-C1B	-2.00	104.91	106.41

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	800	HEM	C2C-C3C-CAC-CBC
2	B	800	HEM	C2C-C3C-CAC-CBC
2	B	800	HEM	C4C-C3C-CAC-CBC
2	D	800	HEM	C2C-C3C-CAC-CBC
3	A	503	PN0	N3-C16-C2-N1
3	B	503	PN0	N3-C16-C2-N1
2	B	800	HEM	C2B-C3B-CAB-CBB
2	A	800	HEM	C4C-C3C-CAC-CBC
2	D	800	HEM	C4C-C3C-CAC-CBC
3	B	503	PN0	C3-N1-S2-O3
3	D	503	PN0	N3-C16-C2-N1
3	A	503	PN0	C3-N1-S2-O3
3	A	503	PN0	O5-C16-C2-N1
3	B	503	PN0	O5-C16-C2-N1
2	C	800	HEM	C2C-C3C-CAC-CBC
2	D	800	HEM	C2B-C3B-CAB-CBB
2	B	800	HEM	C4B-C3B-CAB-CBB
3	D	503	PN0	C3-N1-S2-O3
3	B	503	PN0	C3-N1-S2-O2
3	C	503	PN0	C3-N1-S2-O3
3	D	503	PN0	O5-C16-C2-N1
3	A	503	PN0	C3-N1-S2-O2
3	C	503	PN0	C3-N1-S2-O2
3	D	503	PN0	C3-N1-S2-O2
2	C	800	HEM	C4C-C3C-CAC-CBC
2	C	800	HEM	CAA-CBA-CGA-O2A
3	C	503	PN0	N3-C16-C2-N1
2	C	800	HEM	CAA-CBA-CGA-O1A
3	A	503	PN0	C10-C5-S2-O2
3	B	503	PN0	C10-C5-S2-O2
3	D	503	PN0	C10-C5-S2-O2
3	A	503	PN0	C6-C5-S2-O2
2	B	800	HEM	CAA-CBA-CGA-O2A
3	D	503	PN0	C6-C5-S2-O2
2	A	800	HEM	CAA-CBA-CGA-O2A
3	B	503	PN0	C6-C5-S2-O2

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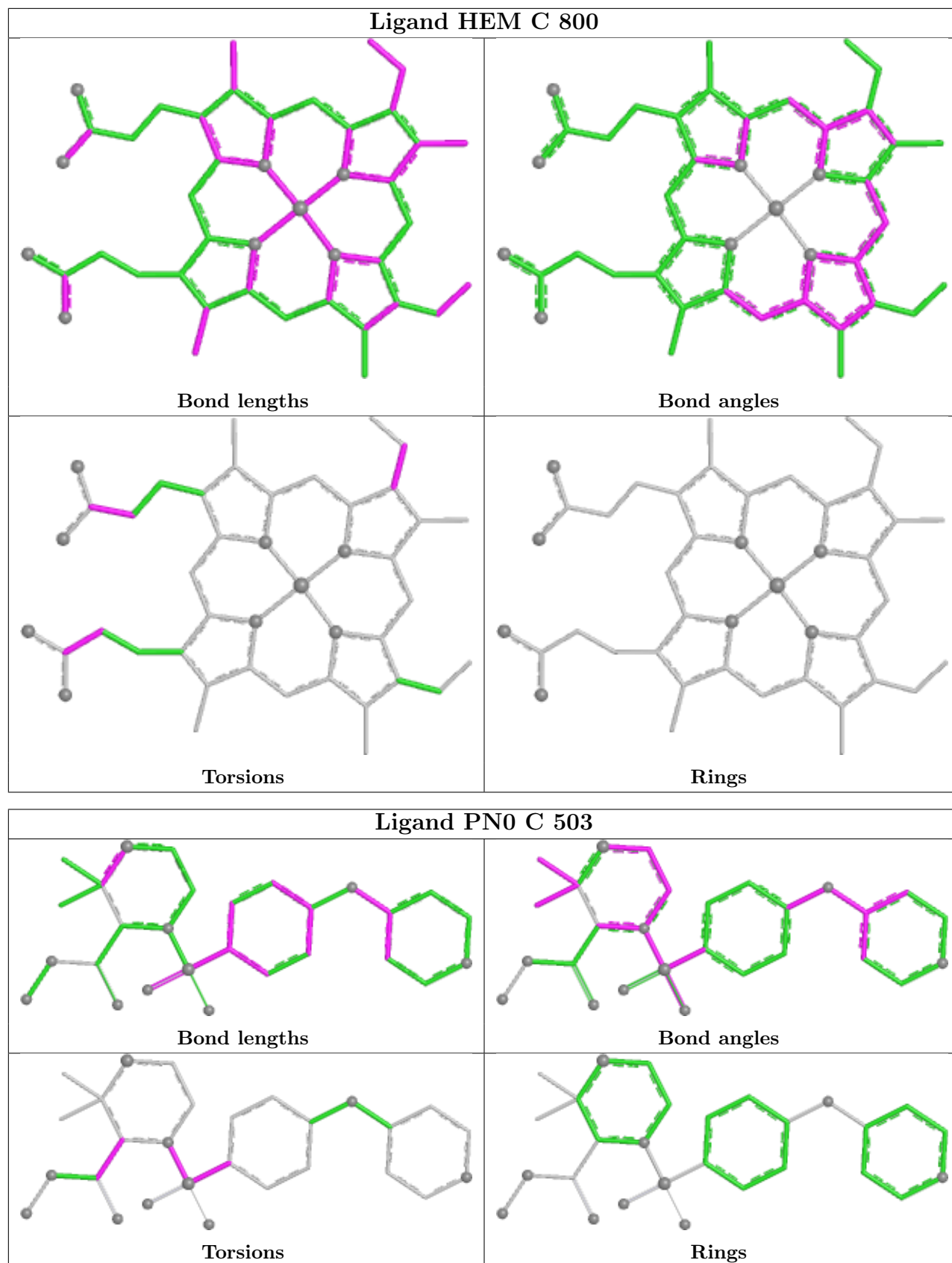
Mol	Chain	Res	Type	Atoms
3	C	503	PN0	C10-C5-S2-O2
2	D	800	HEM	CAA-CBA-CGA-O2A
2	B	800	HEM	CAA-CBA-CGA-O1A
2	A	800	HEM	CAA-CBA-CGA-O1A
3	C	503	PN0	O5-C16-C2-N1
2	D	800	HEM	C4B-C3B-CAB-CBB
2	D	800	HEM	CAA-CBA-CGA-O1A
3	C	503	PN0	C6-C5-S2-O2
3	B	503	PN0	C3-N1-S2-C5
3	A	503	PN0	O5-C16-C2-C1
3	B	503	PN0	O5-C16-C2-C1
2	A	800	HEM	CAD-CBD-CGD-O2D
2	B	800	HEM	CAD-CBD-CGD-O2D
2	C	800	HEM	CAD-CBD-CGD-O2D
3	A	503	PN0	C3-N1-S2-C5
2	C	800	HEM	CAD-CBD-CGD-O1D
2	D	800	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

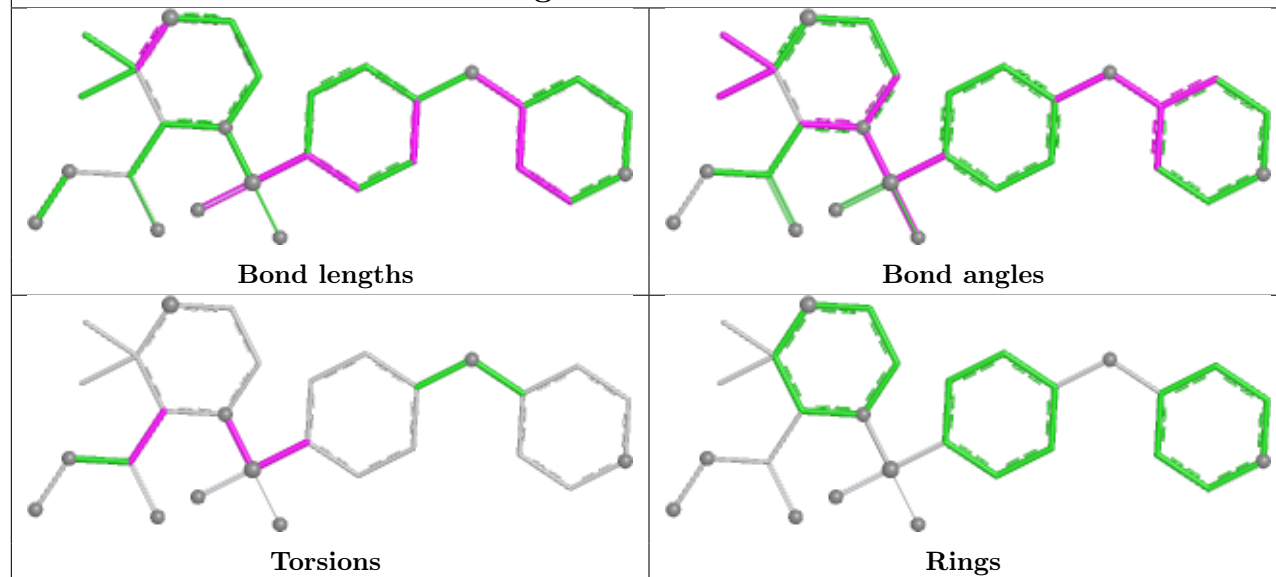
7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	800	HEM	6	0
3	C	503	PN0	1	0
2	B	800	HEM	2	0
2	A	800	HEM	4	0
2	D	800	HEM	3	0
3	D	503	PN0	1	0
3	A	503	PN0	3	0

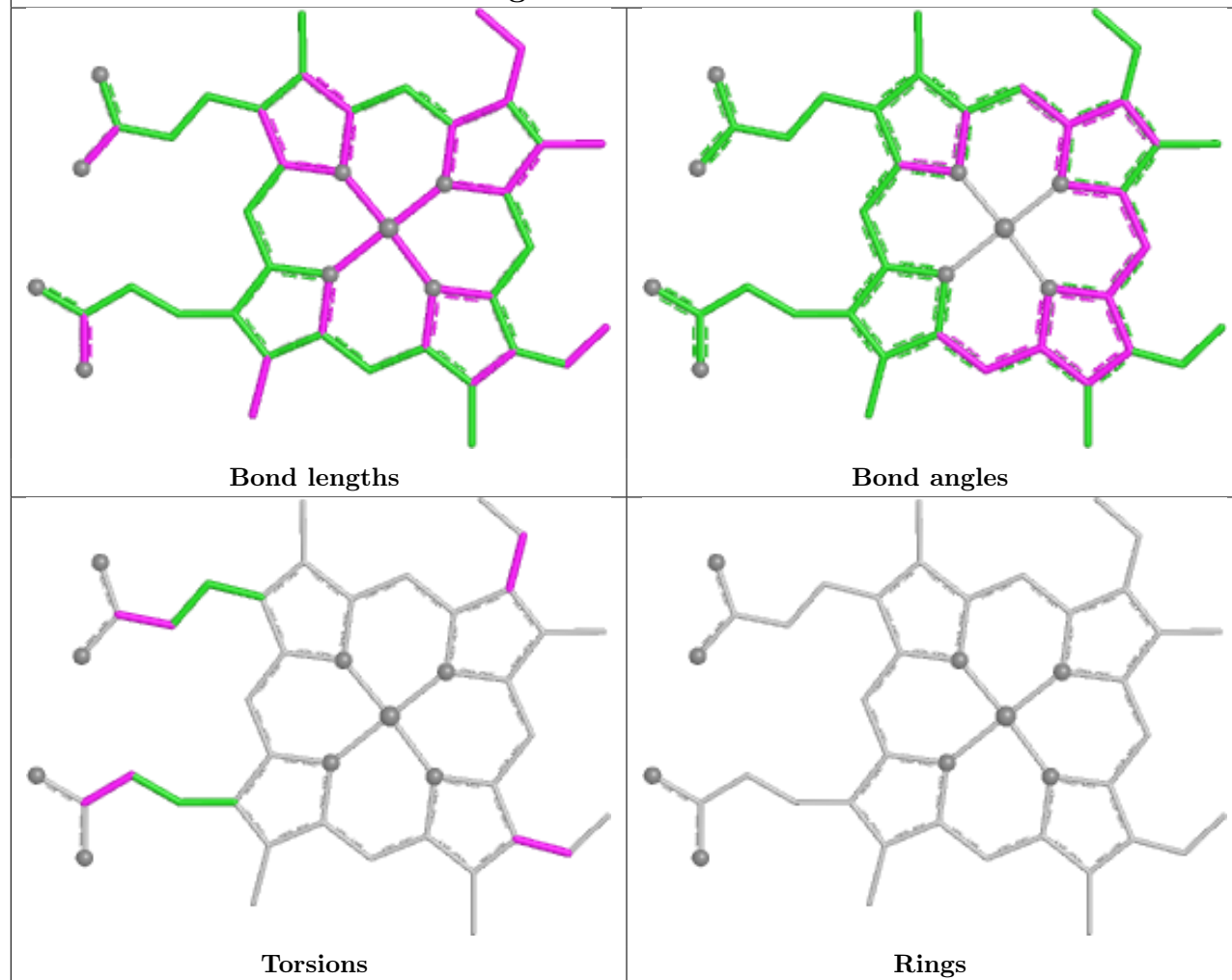
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

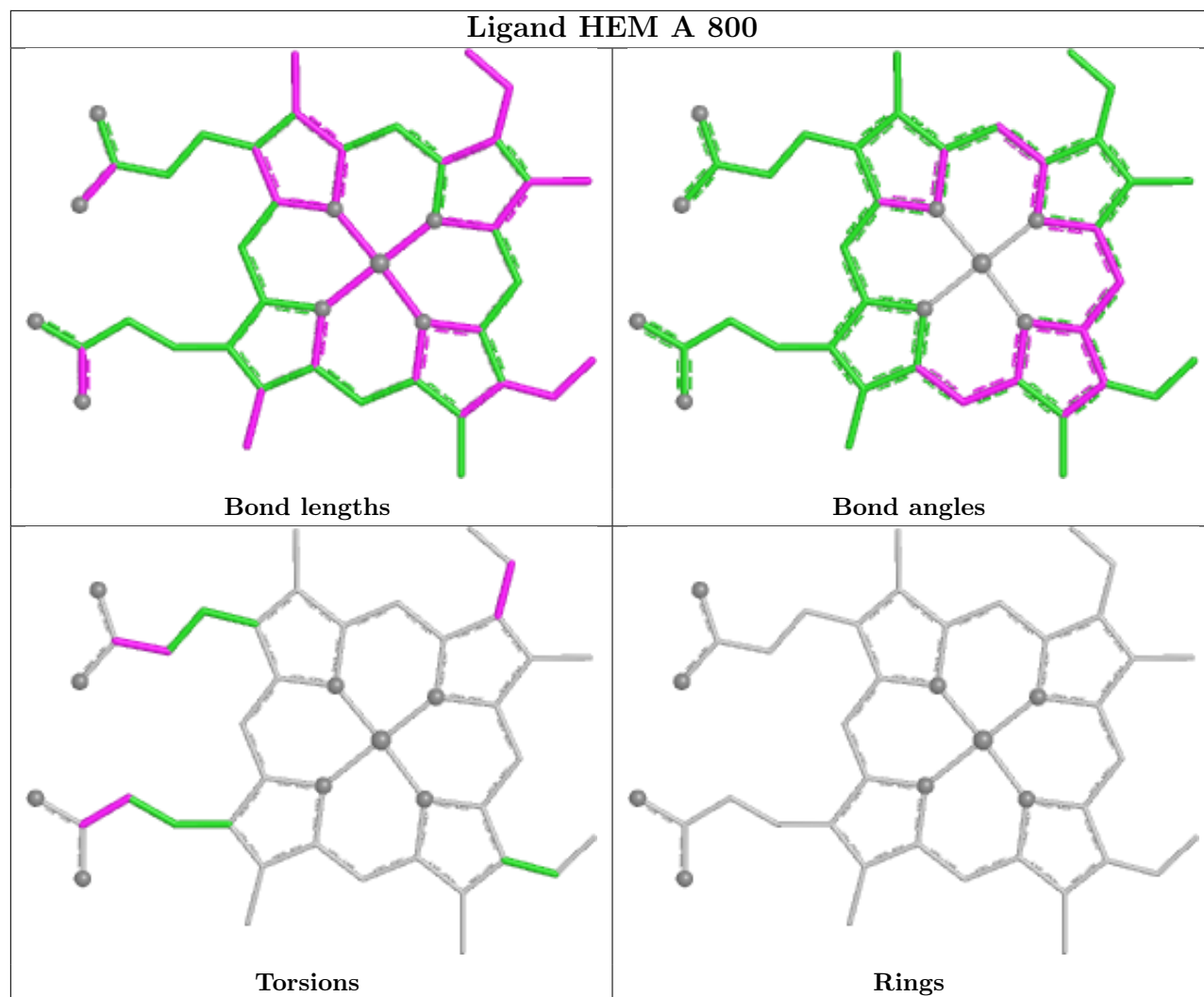


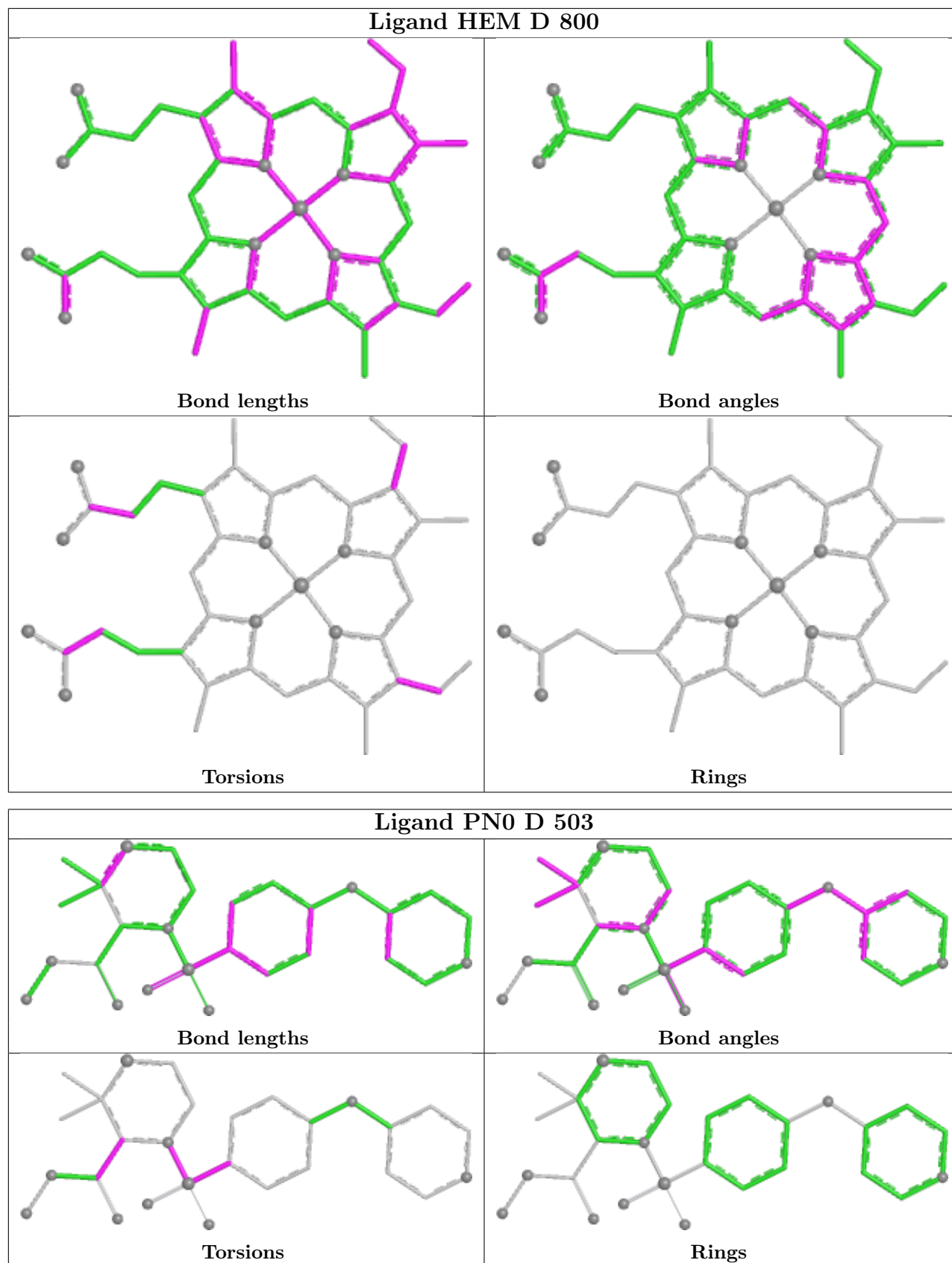
Ligand PN0 B 503

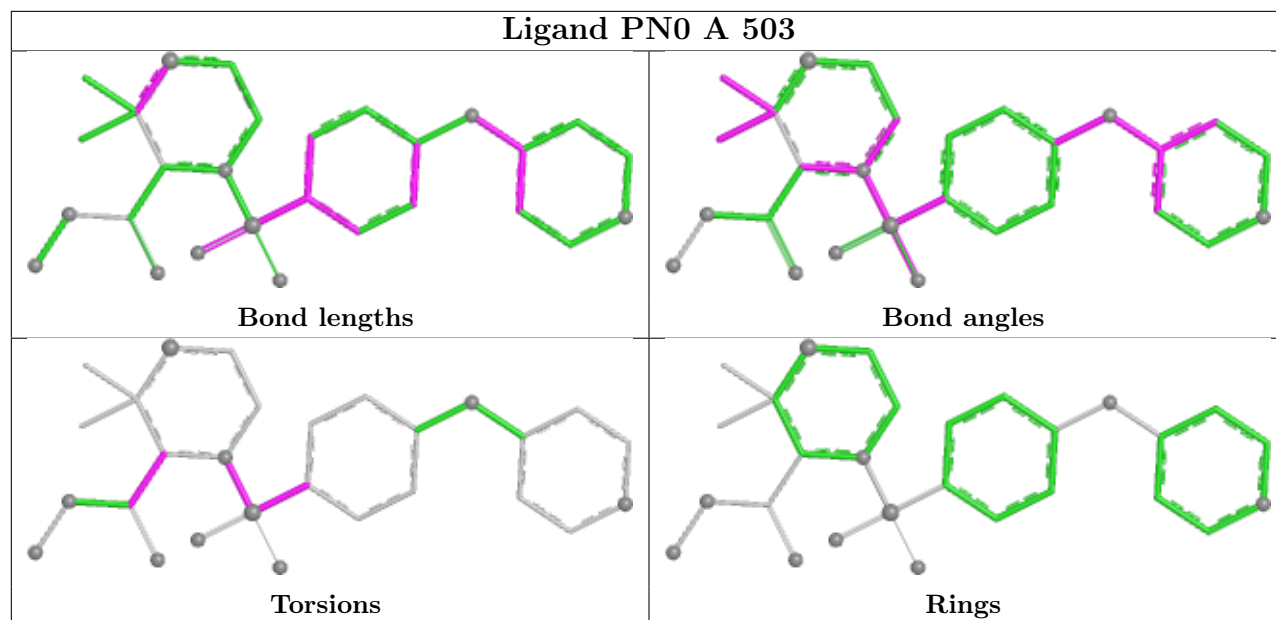


Ligand HEM B 800









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	467/479 (97%)	0.12	25 (5%)	31	27	17, 36, 79, 91	1 (0%)
1	B	456/479 (95%)	0.36	36 (7%)	18	15	25, 42, 87, 100	0
1	C	467/479 (97%)	0.25	41 (8%)	15	13	18, 37, 87, 107	1 (0%)
1	D	456/479 (95%)	0.37	39 (8%)	16	13	25, 44, 83, 96	0
All	All	1846/1916 (96%)	0.27	141 (7%)	20	17	17, 40, 84, 107	2 (0%)

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	477	HIS	7.8
1	C	477	HIS	6.8
1	D	145	GLY	5.6
1	D	39	PRO	5.5
1	B	39	PRO	5.1
1	B	145	GLY	5.1
1	C	145	GLY	4.7
1	D	75	TRP	4.7
1	A	342	VAL	4.6
1	C	342	VAL	4.6
1	B	75	TRP	4.4
1	D	32	LYS	4.3
1	C	40	LEU	4.2
1	D	38	LEU	4.2
1	A	145	GLY	4.2
1	C	43	LEU	4.2
1	A	38	LEU	4.1
1	C	38	LEU	4.1
1	B	214	LYS	4.0
1	D	51	PHE	4.0
1	A	219	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	63	ARG	3.8
1	C	47	LEU	3.8
1	A	214	LYS	3.8
1	B	51	PHE	3.8
1	C	75	TRP	3.7
1	D	240	VAL	3.7
1	D	235	ALA	3.7
1	B	219	PHE	3.6
1	B	144	LEU	3.6
1	D	237	ALA	3.5
1	C	220	LEU	3.4
1	C	74	ALA	3.4
1	C	144	LEU	3.3
1	A	47	LEU	3.3
1	C	41	PRO	3.2
1	C	51	PHE	3.2
1	B	38	LEU	3.2
1	C	39	PRO	3.2
1	A	217	SER	3.2
1	B	235	ALA	3.1
1	B	217	SER	3.1
1	D	307	MET	3.1
1	C	229	VAL	3.1
1	A	144	LEU	3.1
1	C	48	HIS	3.1
1	C	31	GLY	3.1
1	B	32	LYS	3.0
1	D	147	LYS	3.0
1	B	231	LEU	3.0
1	D	220	LEU	3.0
1	D	63	ARG	3.0
1	C	219	PHE	3.0
1	C	46	LEU	2.9
1	D	219	PHE	2.9
1	B	218	GLY	2.9
1	C	169	GLY	2.9
1	D	54	THR	2.9
1	C	463	HIS	2.9
1	A	341	GLN	2.9
1	B	463	HIS	2.9
1	B	216	GLU	2.8
1	D	50	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	144	LEU	2.8
1	D	236	LEU	2.8
1	D	168	SER	2.7
1	D	233	ILE	2.7
1	B	232	HIS	2.7
1	B	229	VAL	2.7
1	D	76	THR	2.7
1	C	44	GLY	2.7
1	B	480	VAL	2.7
1	B	230	LEU	2.6
1	D	231	LEU	2.6
1	A	215	GLU	2.6
1	B	168	SER	2.6
1	D	234	PRO	2.6
1	A	146	LYS	2.6
1	B	169	GLY	2.6
1	C	227	VAL	2.6
1	C	341	GLN	2.6
1	A	463	HIS	2.6
1	A	216	GLU	2.6
1	B	96	GLU	2.6
1	C	45	ASN	2.6
1	D	37	PRO	2.6
1	B	60	GLN	2.6
1	A	231	LEU	2.5
1	D	146	LYS	2.5
1	C	218	GLY	2.5
1	B	215	GLU	2.5
1	A	218	GLY	2.5
1	D	229	VAL	2.5
1	A	75	TRP	2.5
1	B	56	TYR	2.5
1	A	233	ILE	2.4
1	C	239	LYS	2.4
1	A	43	LEU	2.4
1	B	52	GLN	2.4
1	C	482	ALA	2.4
1	A	40	LEU	2.4
1	A	41	PRO	2.4
1	C	340	GLY	2.4
1	B	233	ILE	2.4
1	D	33	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	238	GLY	2.4
1	A	213	LEU	2.3
1	D	230	LEU	2.3
1	D	463	HIS	2.3
1	B	50	ASP	2.3
1	C	168	SER	2.3
1	D	74	ALA	2.3
1	C	151	GLN	2.3
1	C	230	LEU	2.3
1	C	234	PRO	2.3
1	D	148	SER	2.3
1	B	146	LYS	2.2
1	C	147	LYS	2.2
1	C	152	TRP	2.2
1	C	240	VAL	2.2
1	C	307	MET	2.2
1	B	54	THR	2.2
1	A	220	LEU	2.2
1	D	480	VAL	2.2
1	C	235	ALA	2.1
1	B	228	PRO	2.1
1	D	239	LYS	2.1
1	C	217	SER	2.1
1	B	74	ALA	2.1
1	C	32	LYS	2.1
1	B	64	ARG	2.1
1	D	225	ASN	2.1
1	A	482	ALA	2.1
1	B	61	LEU	2.1
1	D	224	LEU	2.1
1	B	53	ASN	2.1
1	D	169	GLY	2.1
1	D	34	PRO	2.0
1	D	71	LEU	2.0
1	C	166	ASN	2.0
1	A	44	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

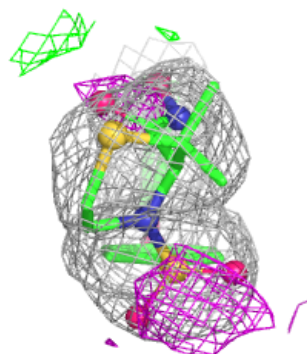
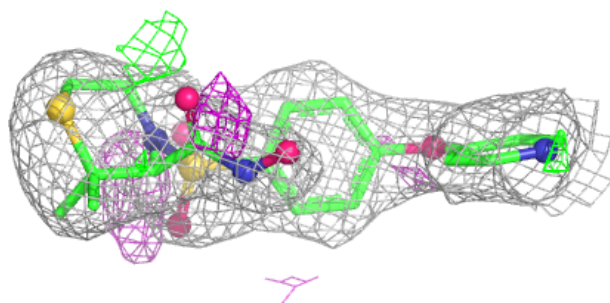
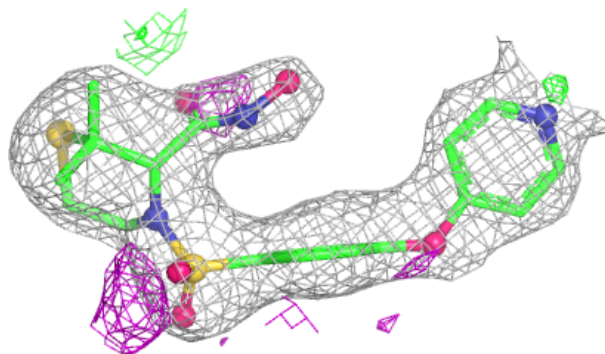
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	PN0	A	503	28/28	0.93	0.12	35,48,53,55	0
3	PN0	B	503	28/28	0.93	0.12	40,48,51,54	0
3	PN0	C	503	28/28	0.94	0.11	36,45,51,55	0
3	PN0	D	503	28/28	0.94	0.11	40,50,52,54	0
2	HEM	A	800	43/43	0.98	0.06	16,21,25,26	0
2	HEM	B	800	43/43	0.98	0.07	23,27,30,34	0
2	HEM	C	800	43/43	0.98	0.06	14,19,23,25	0
2	HEM	D	800	43/43	0.98	0.07	23,25,28,32	0
4	ZN	A	601	1/1	0.99	0.03	34,34,34,34	0
4	ZN	A	600	1/1	1.00	0.01	29,29,29,29	0
4	ZN	B	600	1/1	1.00	0.02	29,29,29,29	0
4	ZN	C	600	1/1	1.00	0.01	35,35,35,35	0
4	ZN	D	600	1/1	1.00	0.02	33,33,33,33	0

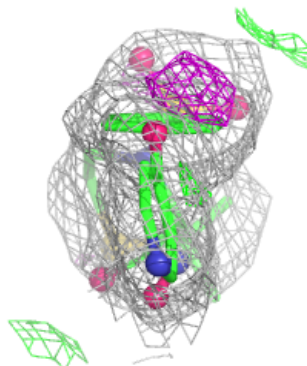
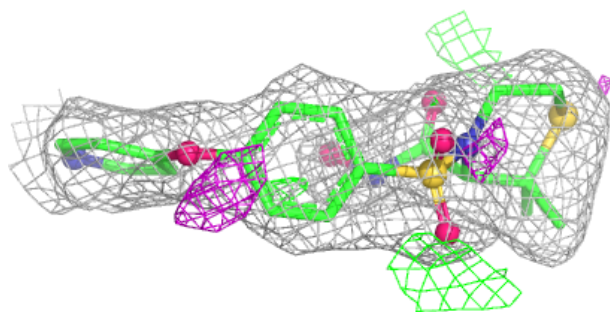
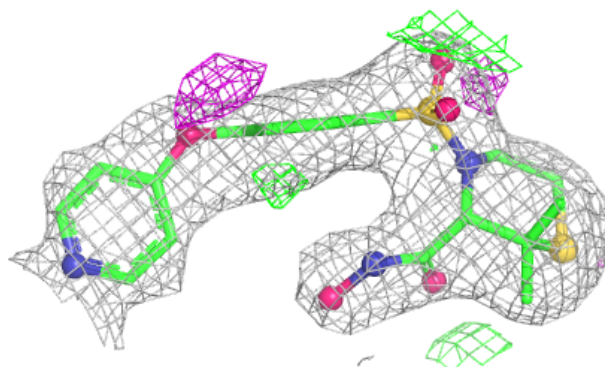
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PN0 A 503:

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

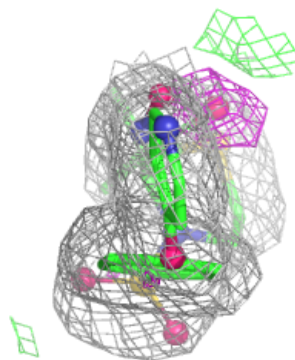
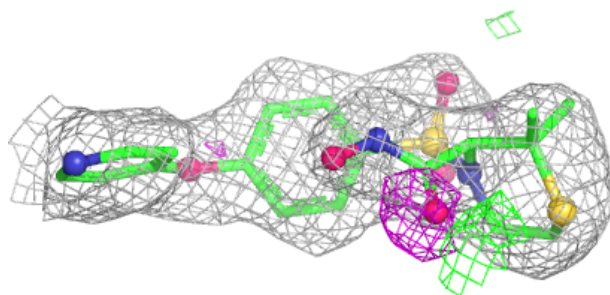
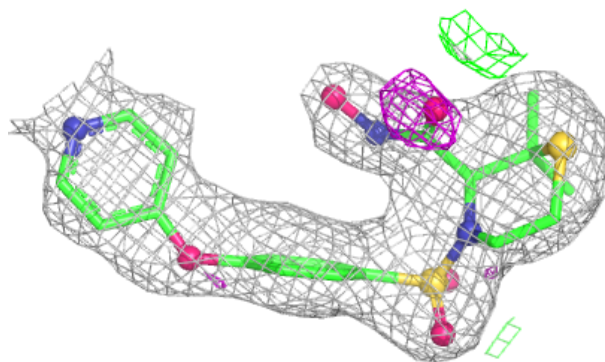
**Electron density around PN0 B 503:**

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

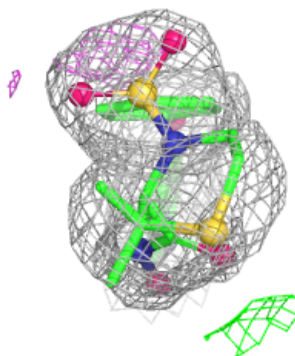
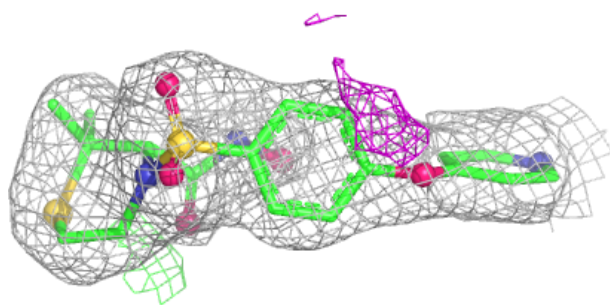
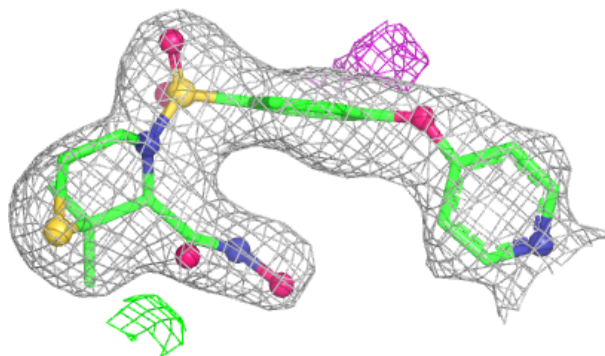


Electron density around PN0 C 503:

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

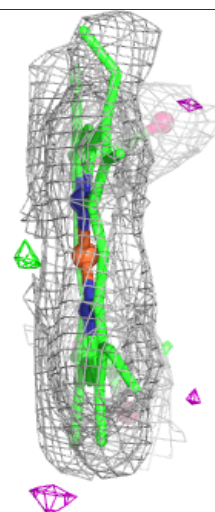
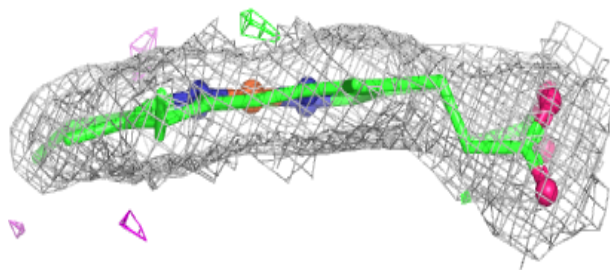
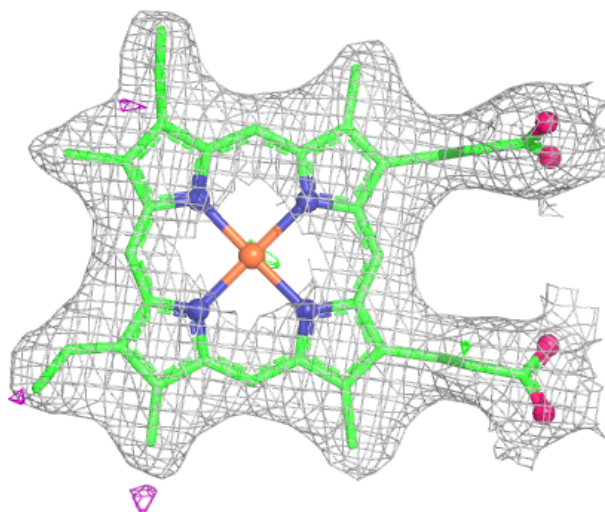
**Electron density around PN0 D 503:**

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



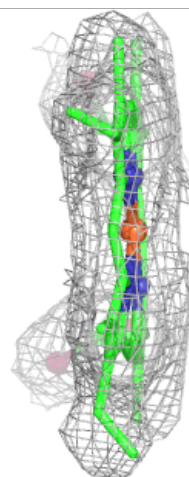
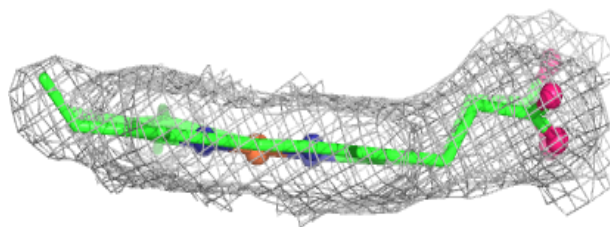
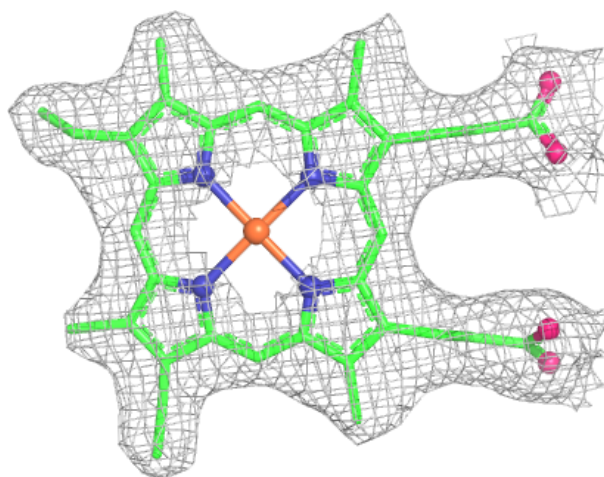
Electron density around HEM A 800:

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



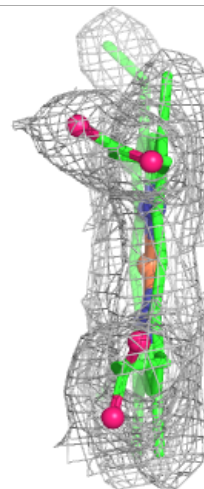
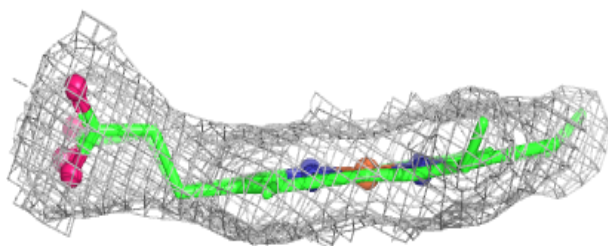
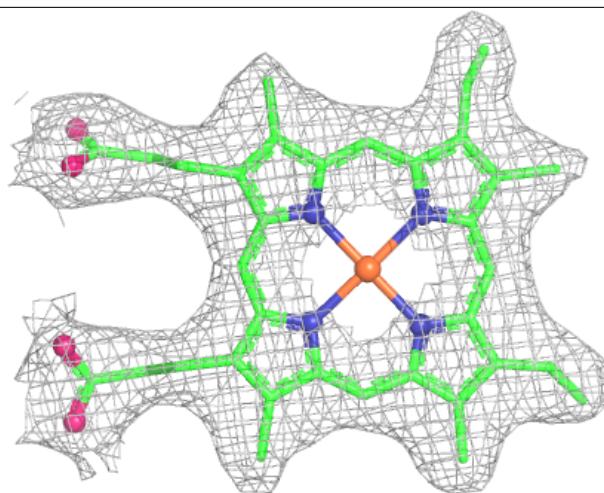
Electron density around HEM B 800:

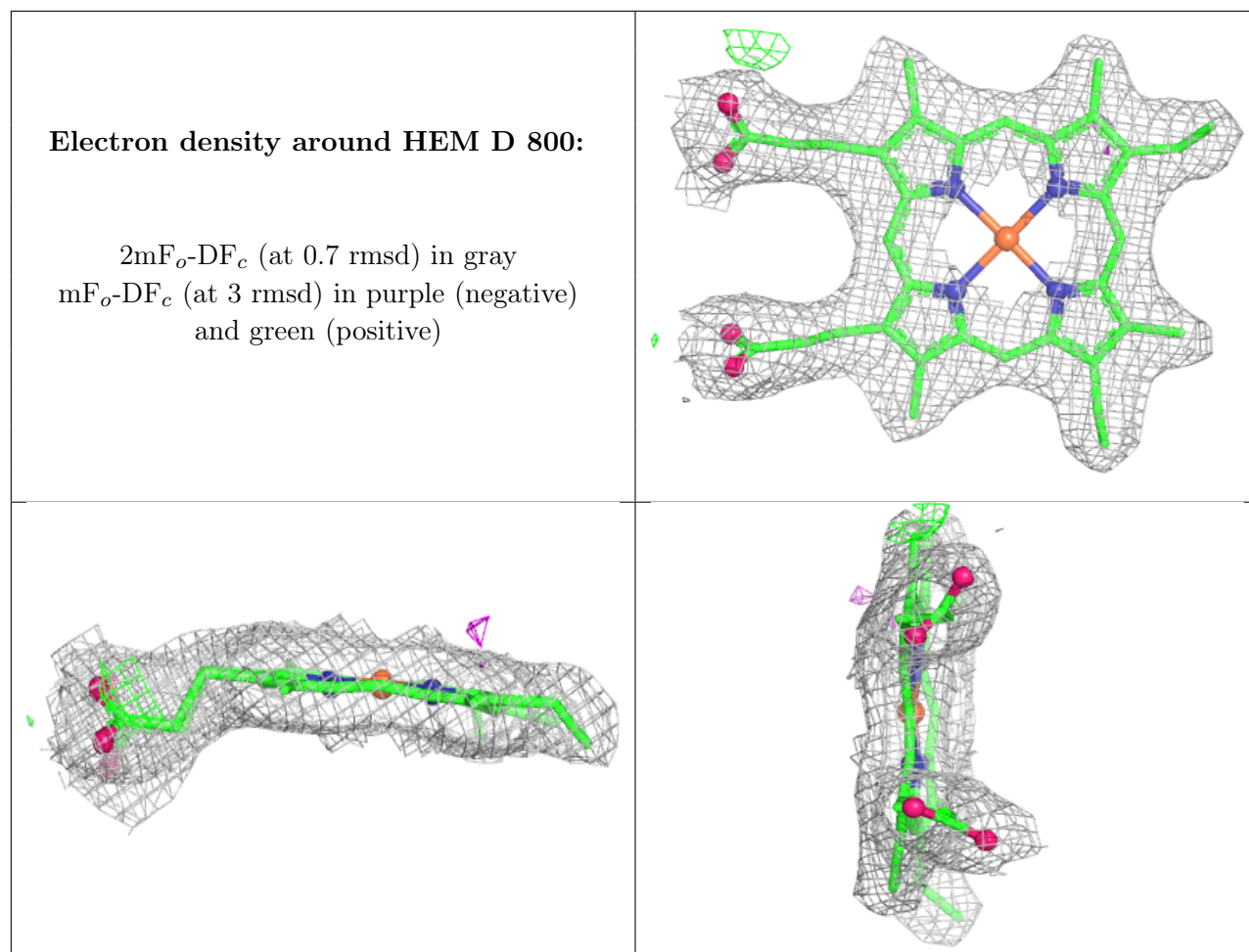
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 800:

$2mF_o-DF_c$ (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.