



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:07 AM UTC

PDB ID : 4EJJ / pdb_00004ejj
Title : Human Cytochrome P450 2A6 in complex with nicotine
Authors : DeVore, N.M.; Scott, E.E.
Deposited on : 2012-04-06
Resolution : 2.30 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

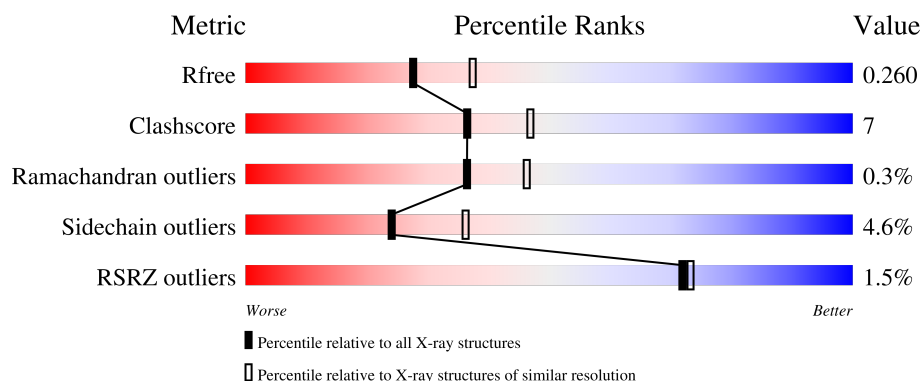
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	81% 15% ..
1	B	476	82% 15% ..
1	C	476	78% 17% ..
1	D	476	73% 22% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NCT	B	501	-	-	X	-
3	NCT	C	501	-	-	X	-
3	NCT	D	501	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15429 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	3	0
			3780	2427	655	680	18			
1	B	464	Total	C	N	O	S	0	2	0
			3762	2416	649	679	18			
1	C	464	Total	C	N	O	S	0	1	0
			3756	2411	648	679	18			
1	D	464	Total	C	N	O	S	0	3	0
			3773	2423	655	677	18			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	initiating methionine	UNP P11509
A	24	ALA	-	expression tag	UNP P11509
A	25	LYS	-	expression tag	UNP P11509
A	26	LYS	-	expression tag	UNP P11509
A	27	THR	-	expression tag	UNP P11509
A	28	SER	-	expression tag	UNP P11509
A	392	TYR	PHE	SEE REMARK 999	UNP P11509
A	495	HIS	-	expression tag	UNP P11509
A	496	HIS	-	expression tag	UNP P11509
A	497	HIS	-	expression tag	UNP P11509
A	498	HIS	-	expression tag	UNP P11509
B	23	MET	-	initiating methionine	UNP P11509
B	24	ALA	-	expression tag	UNP P11509
B	25	LYS	-	expression tag	UNP P11509
B	26	LYS	-	expression tag	UNP P11509
B	27	THR	-	expression tag	UNP P11509
B	28	SER	-	expression tag	UNP P11509
B	392	TYR	PHE	SEE REMARK 999	UNP P11509
B	495	HIS	-	expression tag	UNP P11509
B	496	HIS	-	expression tag	UNP P11509
B	497	HIS	-	expression tag	UNP P11509

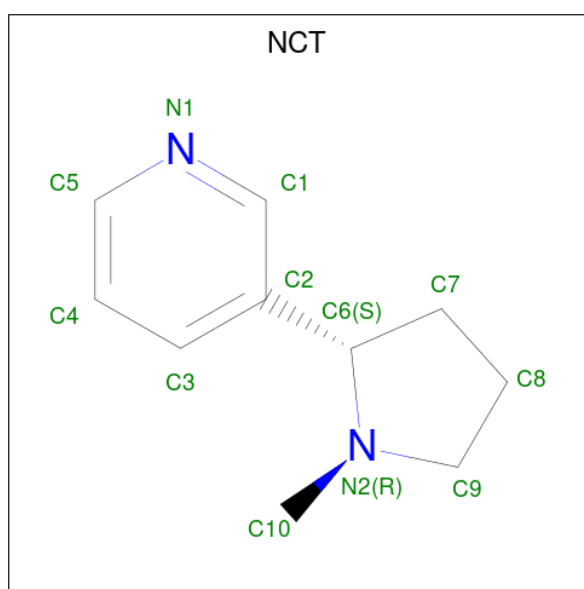
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Chain	Residue	Modelled	Actual	Comment	Reference
B	498	HIS	-	expression tag	UNP P11509
C	23	MET	-	initiating methionine	UNP P11509
C	24	ALA	-	expression tag	UNP P11509
C	25	LYS	-	expression tag	UNP P11509
C	26	LYS	-	expression tag	UNP P11509
C	27	THR	-	expression tag	UNP P11509
C	28	SER	-	expression tag	UNP P11509
C	392	TYR	PHE	SEE REMARK 999	UNP P11509
C	495	HIS	-	expression tag	UNP P11509
C	496	HIS	-	expression tag	UNP P11509
C	497	HIS	-	expression tag	UNP P11509
C	498	HIS	-	expression tag	UNP P11509
D	23	MET	-	initiating methionine	UNP P11509
D	24	ALA	-	expression tag	UNP P11509
D	25	LYS	-	expression tag	UNP P11509
D	26	LYS	-	expression tag	UNP P11509
D	27	THR	-	expression tag	UNP P11509
D	28	SER	-	expression tag	UNP P11509
D	392	TYR	PHE	SEE REMARK 999	UNP P11509
D	495	HIS	-	expression tag	UNP P11509
D	496	HIS	-	expression tag	UNP P11509
D	497	HIS	-	expression tag	UNP P11509
D	498	HIS	-	expression tag	UNP P11509

- # HEM

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

- Molecule 3 is (S)-3-(1-METHYLPYRROLIDIN-2-YL)PYRIDINE (CCD ID: NCT) (formula: $C_{10}H_{14}N_2$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C N	0	0
			12 10 2			
3	B	1	Total	C N	0	0
			12 10 2			
3	C	1	Total	C N	0	0
			12 10 2			
3	D	1	Total	C N	0	0
			12 10 2			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	51	Total O	0	0
			51 51		

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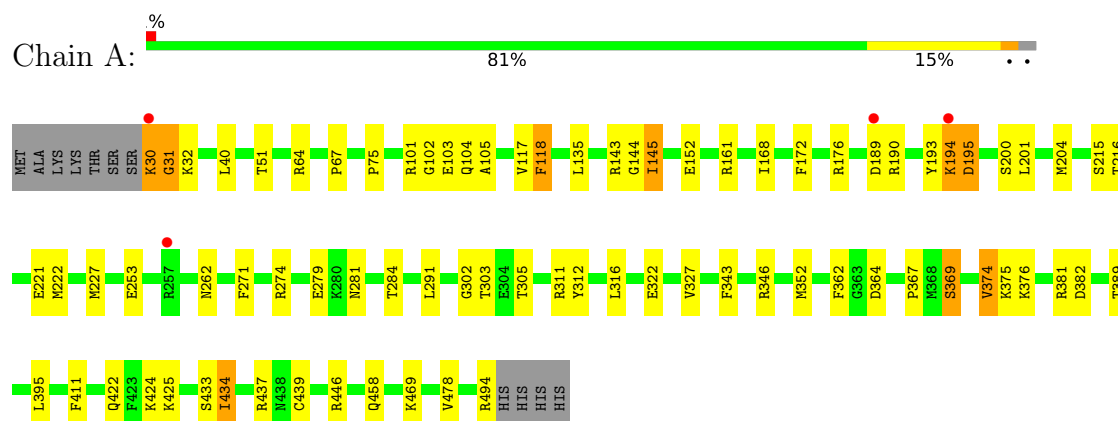
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	29	Total 29	O 29	0	0
4	C	23	Total 23	O 23	0	0
4	D	35	Total 35	O 35	0	0

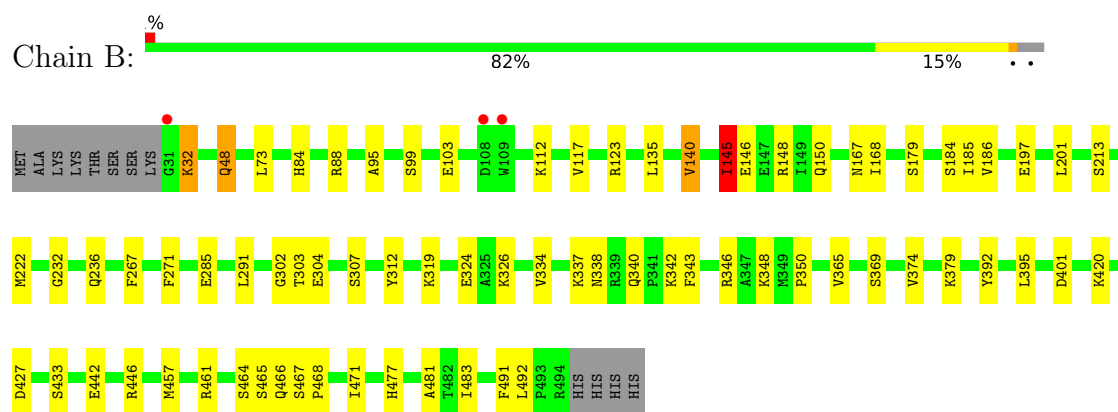
3 Residue-property plots [i](#)

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.

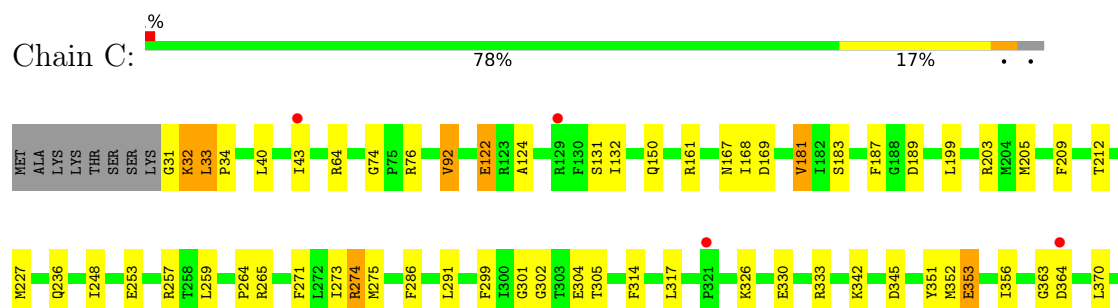
• Molecule 1: Cytochrome P450 2A6

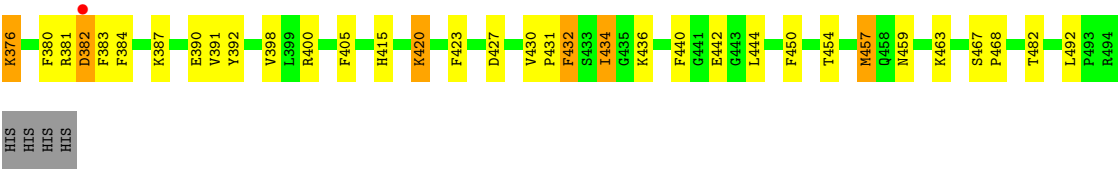


• Molecule 1: Cytochrome P450 2A6

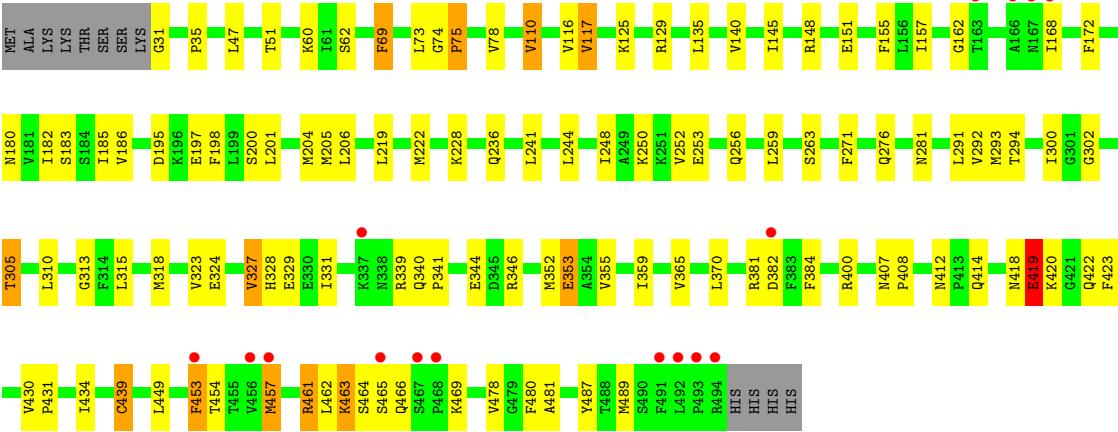


• Molecule 1: Cytochrome P450 2A6





● Molecule 1: Cytochrome P450 2A6



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.21Å 194.04Å 90.27Å 90.00° 102.70° 90.00°	Depositor
Resolution (Å)	97.02 – 2.30 97.02 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (97.02-2.30) 100.0 (97.02-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.29Å)	Xtriage
Refinement program	REFMAC 6.1.13	Depositor
R, R_{free}	0.203 , 0.264 0.202 , 0.260	Depositor DCC
R_{free} test set	5275 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15429	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.41	14/3880 (0.4%)	1.28	10/5224 (0.2%)
1	B	1.25	3/3859 (0.1%)	1.29	16/5197 (0.3%)
1	C	1.25	7/3850 (0.2%)	1.27	20/5186 (0.4%)
1	D	1.34	12/3873 (0.3%)	1.29	14/5214 (0.3%)
All	All	1.31	36/15462 (0.2%)	1.28	60/20821 (0.3%)

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	75	PRO	CA-C	7.56	1.60	1.52
1	A	216	THR	CA-CB	7.12	1.64	1.53
1	A	75	PRO	C-O	-7.05	1.15	1.24
1	A	369	SER	CA-C	6.87	1.61	1.52
1	B	374	VAL	CA-CB	6.79	1.62	1.54
1	A	434	ILE	CA-CB	6.62	1.63	1.54
1	D	382	ASP	CA-C	6.16	1.62	1.52
1	A	67	PRO	C-O	-6.01	1.17	1.24
1	C	427	ASP	CA-C	5.99	1.60	1.52
1	C	132	ILE	CA-CB	5.94	1.61	1.54
1	A	145	ILE	CA-CB	5.89	1.62	1.54
1	A	221	GLU	C-O	-5.85	1.17	1.24
1	A	312	TYR	C-O	-5.84	1.17	1.24
1	D	439	CYS	C-O	-5.81	1.17	1.24
1	D	186	VAL	CA-CB	5.79	1.61	1.54
1	C	264	PRO	CA-C	5.65	1.57	1.52
1	C	391	VAL	CA-CB	5.60	1.61	1.54
1	C	150	GLN	N-CA	5.58	1.53	1.46
1	A	422	GLN	CA-C	5.51	1.59	1.52
1	A	478	VAL	C-O	-5.47	1.18	1.24
1	A	311	ARG	C-O	-5.46	1.17	1.24
1	D	292	VAL	CA-CB	5.42	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	31	GLY	N-CA	5.34	1.54	1.45
1	A	303	THR	CA-C	5.24	1.57	1.52
1	A	102	GLY	C-O	-5.23	1.18	1.23
1	B	140	VAL	CA-CB	5.21	1.59	1.54
1	D	145	ILE	CA-CB	5.21	1.60	1.54
1	D	228	LYS	CA-C	5.19	1.60	1.52
1	A	104	GLN	C-O	-5.17	1.18	1.24
1	B	32	LYS	CA-C	5.12	1.58	1.52
1	C	380	PHE	CA-C	5.11	1.58	1.52
1	D	384	PHE	N-CA	-5.11	1.40	1.46
1	D	110	VAL	CA-C	5.09	1.59	1.52
1	D	292	VAL	CA-C	5.08	1.59	1.52
1	D	140	VAL	CA-CB	5.06	1.60	1.54
1	C	212	THR	CA-CB	5.04	1.62	1.53

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	92	VAL	CB-CA-C	8.53	118.96	111.71
1	C	64	ARG	N-CA-C	8.49	120.31	111.14
1	C	382	ASP	CB-CA-C	-7.17	102.73	109.83
1	B	304	GLU	N-CA-C	7.07	119.07	111.36
1	B	483	ILE	CA-C-N	-6.93	113.52	120.31
1	B	483	ILE	C-N-CA	-6.93	113.52	120.31
1	D	74	GLY	CA-C-N	-6.79	113.12	121.00
1	D	74	GLY	C-N-CA	-6.79	113.12	121.00
1	D	461	ARG	N-CA-C	-6.73	98.86	109.50
1	D	47	LEU	N-CA-C	6.72	119.44	111.71
1	D	327	VAL	N-CA-C	-6.63	104.39	110.82
1	D	157	ILE	N-CA-C	6.56	116.71	110.42
1	C	398	VAL	N-CA-C	-6.53	104.49	110.82
1	A	362	PHE	CA-C-N	6.35	126.99	119.94
1	A	362	PHE	C-N-CA	6.35	126.99	119.94
1	A	281	ASN	CA-C-N	-6.28	113.71	121.00
1	A	281	ASN	C-N-CA	-6.28	113.71	121.00
1	A	478	VAL	CB-CA-C	-6.26	101.19	110.33
1	C	436	LYS	N-CA-C	6.21	118.84	111.71
1	B	340	GLN	CA-C-N	-6.16	113.44	119.78
1	B	340	GLN	C-N-CA	-6.16	113.44	119.78
1	D	419	GLU	N-CA-C	5.82	117.31	110.97
1	C	265	ARG	N-CA-C	5.74	117.62	111.36
1	B	145	ILE	N-CA-C	5.73	116.51	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	ILE	N-CA-C	5.70	115.89	110.53
1	C	304	GLU	N-CA-C	5.69	117.56	111.36
1	C	131	SER	N-CA-C	5.68	117.15	111.07
1	C	432	PHE	N-CA-C	-5.66	105.72	113.30
1	C	492	LEU	CA-C-N	5.63	125.65	119.90
1	C	492	LEU	C-N-CA	5.63	125.65	119.90
1	C	227	MET	N-CA-C	5.59	118.30	111.82
1	B	374	VAL	N-CA-CB	5.58	116.61	110.53
1	B	232	GLY	CA-C-N	5.55	125.38	119.28
1	B	232	GLY	C-N-CA	5.55	125.38	119.28
1	B	32	LYS	N-CA-C	5.53	118.24	109.50
1	A	446	ARG	N-CA-C	-5.49	105.45	111.82
1	B	184	SER	N-CA-C	-5.46	105.49	111.82
1	D	293	MET	N-CA-C	5.45	117.30	111.36
1	C	382	ASP	N-CA-CB	-5.42	108.68	114.10
1	B	334	VAL	N-CA-C	5.42	118.70	111.44
1	C	169	ASP	CA-C-N	-5.37	115.36	120.83
1	C	169	ASP	C-N-CA	-5.37	115.36	120.83
1	C	124	ALA	N-CA-C	5.35	117.55	111.02
1	A	117	VAL	N-CA-C	5.27	115.48	110.42
1	D	381	ARG	CA-C-N	-5.26	114.79	123.05
1	D	381	ARG	C-N-CA	-5.26	114.79	123.05
1	D	69	PHE	N-CA-C	5.26	116.80	108.96
1	C	189	ASP	N-CA-C	5.19	116.17	108.60
1	C	392	TYR	CA-C-N	-5.17	113.37	119.84
1	C	392	TYR	C-N-CA	-5.17	113.37	119.84
1	A	118	PHE	N-CA-C	5.14	119.19	113.02
1	D	281	ASN	CA-C-N	-5.08	114.81	120.45
1	D	281	ASN	C-N-CA	-5.08	114.81	120.45
1	B	338	ASN	N-CA-C	5.07	119.33	112.04
1	C	259	LEU	N-CA-C	5.06	117.00	109.25
1	A	227	MET	N-CA-C	5.06	117.53	111.71
1	A	105	ALA	N-CA-C	5.04	116.86	111.36
1	D	117	VAL	N-CA-C	5.02	115.23	110.42
1	B	392	TYR	CA-C-N	-5.01	114.28	120.79
1	B	392	TYR	C-N-CA	-5.01	114.28	120.79

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	3780	0	3776	42	0
1	B	3762	0	3751	43	0
1	C	3756	0	3738	55	0
1	D	3773	0	3773	64	0
2	A	43	0	30	4	0
2	B	43	0	30	9	0
2	C	43	0	30	8	0
2	D	43	0	30	6	0
3	A	12	0	14	3	0
3	B	12	0	14	6	0
3	C	12	0	14	6	0
3	D	12	0	14	6	0
4	A	51	0	0	4	0
4	B	29	0	0	3	0
4	C	23	0	0	0	0
4	D	35	0	0	2	0
All	All	15429	0	15214	220	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 7.

All (220) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:501:NCT:H102	3:B:501:NCT:C1	1.66	1.16
3:B:501:NCT:HC1	3:B:501:NCT:C10	1.75	1.16
1:D:419:GLU:OE2	1:D:419:GLU:HA	1.42	1.09
1:C:381:ARG:O	1:C:382:ASP:HB2	1.43	1.07
1:C:43:ILE:O	1:C:74:GLY:HA2	1.52	1.06
3:B:501:NCT:C1	3:B:501:NCT:C10	2.32	0.98
1:C:457:MET:HA	1:C:457:MET:HE2	1.43	0.97
1:B:103:GLU:HG2	4:B:614:HOH:O	1.69	0.91
1:B:112:LYS:HE2	4:B:629:HOH:O	1.73	0.89
1:D:302:GLY:HA2	2:D:502:HEM:HMC3	1.54	0.89
3:B:501:NCT:H102	3:B:501:NCT:HC1	0.90	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LYS:O	1:A:31:GLY:O	1.92	0.88
1:D:252:VAL:O	1:D:256:GLN:HG3	1.73	0.88
3:A:501:NCT:H102	3:A:501:NCT:HC3	1.57	0.86
1:C:302:GLY:HA2	2:C:500:HEM:HMC2	1.59	0.84
1:A:343:PHE:O	1:A:346:ARG:HB2	1.84	0.77
2:C:500:HEM:C4A	3:C:501:NCT:HC81	2.20	0.76
1:C:43:ILE:O	1:C:74:GLY:CA	2.33	0.76
2:C:500:HEM:NA	3:C:501:NCT:HC81	2.01	0.76
1:C:199:LEU:HD21	1:C:203:ARG:HH21	1.52	0.75
1:A:51:THR:HG22	1:A:222:MET:CE	2.19	0.73
1:D:453:PHE:O	1:D:457:MET:HG2	1.88	0.72
1:C:457:MET:HA	1:C:457:MET:CE	2.18	0.72
1:B:461:ARG:HH12	1:B:492:LEU:HD13	1.54	0.71
1:C:342:LYS:O	1:C:345:ASP:HB2	1.90	0.70
1:B:319:LYS:HD2	1:B:468:PRO:O	1.91	0.70
2:B:500:HEM:C1D	3:B:501:NCT:H101	2.26	0.69
1:D:352:MET:HE3	1:D:454:THR:OG1	1.92	0.69
1:C:381:ARG:O	1:C:382:ASP:CB	2.29	0.69
1:D:419:GLU:OE2	1:D:419:GLU:CA	2.28	0.69
1:A:494:ARG:C	4:A:613:HOH:O	2.36	0.68
1:B:302:GLY:HA2	2:B:500:HEM:HMC3	1.74	0.68
1:D:197:GLU:HG2	4:D:607:HOH:O	1.93	0.68
1:C:302:GLY:HA2	2:C:500:HEM:CMC	2.23	0.68
1:D:418:ASN:OD1	1:D:418:ASN:C	2.38	0.67
1:D:305:THR:HG21	3:D:501:NCT:HC92	1.76	0.67
1:A:189:ASP:OD1	1:A:190:ARG:N	2.30	0.64
1:A:302:GLY:HA2	2:A:500:HEM:HMC3	1.77	0.64
1:A:271:PHE:CD2	1:A:291:LEU:HB2	2.32	0.64
2:D:502:HEM:HMB1	2:D:502:HEM:HBB2	1.79	0.64
1:A:161:ARG:NH2	1:C:420:LYS:CD	2.60	0.64
1:D:148:ARG:NH2	1:D:151:GLU:OE1	2.29	0.64
1:D:248:ILE:O	1:D:252:VAL:HG23	1.99	0.63
1:D:480:PHE:HZ	3:D:501:NCT:H103	1.63	0.63
1:B:433:SER:HB3	2:B:500:HEM:HBA1	1.81	0.62
1:B:179:SER:HB2	1:B:303:THR:HG23	1.80	0.62
1:A:161:ARG:NH2	1:C:420:LYS:HD2	2.14	0.62
1:A:364:ASP:OD2	1:A:367:PRO:HB3	1.99	0.62
3:A:501:NCT:HC3	3:A:501:NCT:C10	2.28	0.62
1:C:301:GLY:HA2	3:C:501:NCT:H103	1.82	0.61
1:D:331:ILE:HD11	1:D:352:MET:HE1	1.82	0.61
1:C:31:GLY:HA3	1:C:384:PHE:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:ARG:NH1	1:B:492:LEU:HD13	2.15	0.61
3:A:501:NCT:C10	3:A:501:NCT:C3	2.78	0.61
1:A:176:ARG:HD2	1:A:193:TYR:CD1	2.36	0.60
1:B:468:PRO:HA	1:B:471:ILE:HD12	1.83	0.60
1:B:103:GLU:CG	4:B:614:HOH:O	2.37	0.60
1:D:302:GLY:HA2	2:D:502:HEM:CMC	2.29	0.60
2:C:500:HEM:C1A	3:C:501:NCT:HC81	2.37	0.60
1:A:274:ARG:HD3	4:A:644:HOH:O	2.02	0.60
1:D:51:THR:HG22	1:D:222:MET:HE3	1.84	0.59
3:D:501:NCT:C10	3:D:501:NCT:HC3	2.32	0.59
1:D:151:GLU:HG2	1:D:155:PHE:CE1	2.38	0.59
1:D:327:VAL:HG12	1:D:331:ILE:HD12	1.84	0.59
1:A:51:THR:HG22	1:A:222:MET:HE3	1.83	0.59
2:B:500:HEM:HBB2	2:B:500:HEM:HMB2	1.84	0.58
1:C:364:ASP:OD2	1:C:400:ARG:NH2	2.36	0.58
1:D:51:THR:HG22	1:D:222:MET:CE	2.33	0.58
1:D:353:GLU:HG2	1:D:423:PHE:CD2	2.39	0.58
1:A:161:ARG:NH2	1:C:420:LYS:HD3	2.19	0.57
1:C:183:SER:O	1:C:187:PHE:HB2	2.04	0.57
1:D:151:GLU:HG2	1:D:155:PHE:HE1	1.69	0.57
1:D:449:LEU:O	1:D:453:PHE:HB2	2.04	0.57
1:C:253:GLU:HB3	1:C:257:ARG:HH12	1.70	0.56
1:A:381:ARG:O	1:A:382:ASP:HB2	2.05	0.56
1:B:369:SER:HB2	1:B:395:LEU:HG	1.87	0.56
1:A:51:THR:HG22	1:A:222:MET:HE1	1.86	0.56
1:A:369:SER:HB2	1:A:395:LEU:HG	1.86	0.56
1:B:123:ARG:HA	1:B:285:GLU:HG3	1.86	0.56
1:A:51:THR:CG2	1:A:222:MET:CE	2.83	0.55
2:B:500:HEM:NA	3:B:501:NCT:HC92	2.21	0.55
1:A:51:THR:CG2	1:A:222:MET:HE1	2.36	0.55
1:C:352:MET:HE3	1:C:454:THR:HA	1.87	0.55
1:D:197:GLU:CG	4:D:607:HOH:O	2.51	0.54
1:C:76:ARG:NH2	1:C:390:GLU:OE2	2.40	0.54
1:D:110:VAL:HG11	1:D:241:LEU:HD22	1.89	0.54
1:A:161:ARG:CZ	1:C:420:LYS:CD	2.87	0.53
1:D:117:VAL:HG22	2:D:502:HEM:HAD1	1.91	0.53
3:D:501:NCT:H103	3:D:501:NCT:HC3	1.90	0.53
1:C:43:ILE:C	1:C:74:GLY:HA2	2.31	0.52
1:D:116:VAL:HG12	1:D:294:THR:HG23	1.91	0.52
1:B:186:VAL:HA	1:B:267:PHE:HB3	1.92	0.52
1:B:461:ARG:NH1	1:B:492:LEU:CD1	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:GLU:O	1:B:446:ARG:HG3	2.10	0.52
1:C:376:LYS:HA	1:C:387:LYS:HG3	1.92	0.52
1:C:271:PHE:CD2	1:C:291:LEU:HB2	2.45	0.51
1:D:62:SER:HB3	1:D:69:PHE:CE2	2.44	0.51
1:D:200:SER:O	1:D:204:MET:HG3	2.09	0.51
1:C:353:GLU:HG2	1:C:423:PHE:CD2	2.45	0.51
1:D:195:ASP:HB3	1:D:198:PHE:HB2	1.93	0.51
1:C:122:GLU:OE2	1:C:122:GLU:HA	2.11	0.51
1:B:140:VAL:HA	1:B:145:ILE:HG21	1.92	0.51
1:D:331:ILE:HD11	1:D:352:MET:CE	2.42	0.50
2:A:500:HEM:HMB1	2:A:500:HEM:HBB2	1.92	0.50
1:D:271:PHE:HB3	1:D:291:LEU:HD13	1.94	0.50
1:B:302:GLY:HA2	2:B:500:HEM:CMC	2.40	0.50
1:D:464:SER:OG	1:D:466:GLN:O	2.29	0.50
1:B:433:SER:CB	2:B:500:HEM:HBA1	2.41	0.50
2:B:500:HEM:HBB2	2:B:500:HEM:CMB	2.42	0.50
1:C:253:GLU:HB3	1:C:257:ARG:NH1	2.25	0.50
2:C:500:HEM:C4D	3:C:501:NCT:HC71	2.47	0.50
1:D:62:SER:HB3	1:D:69:PHE:HE2	1.77	0.50
1:B:150:GLN:NE2	1:B:342:LYS:HB3	2.26	0.49
1:C:92:VAL:HG23	1:C:434:ILE:HD12	1.93	0.49
1:C:405:PHE:HB3	1:C:415:HIS:CD2	2.47	0.49
1:A:322:GLU:HB2	4:A:641:HOH:O	2.11	0.49
1:C:181:VAL:HG11	1:C:444:LEU:HD11	1.95	0.49
2:A:500:HEM:HBB2	2:A:500:HEM:CMB	2.43	0.49
1:D:324:GLU:OE2	1:D:462:LEU:HG	2.11	0.48
1:B:319:LYS:NZ	1:B:471:ILE:O	2.46	0.48
1:D:310:LEU:HA	1:D:453:PHE:CZ	2.49	0.48
1:B:267:PHE:C	1:B:267:PHE:CD2	2.91	0.48
1:C:34:PRO:HA	1:C:383:PHE:CD2	2.49	0.48
1:D:205:MET:HE2	1:D:300:ILE:HG13	1.96	0.48
1:B:117:VAL:HG22	2:B:500:HEM:HAD1	1.96	0.48
1:C:467:SER:O	1:C:468:PRO:C	2.57	0.48
1:D:110:VAL:CG1	1:D:241:LEU:HD22	2.44	0.47
1:A:194:LYS:O	1:A:195:ASP:C	2.57	0.47
1:A:316:LEU:HD13	1:A:411:PHE:CE1	2.49	0.47
1:B:457:MET:HE2	1:B:457:MET:HB3	1.69	0.47
1:C:432:PHE:CD2	1:C:442:GLU:HG3	2.49	0.47
1:B:271:PHE:HB3	1:B:291:LEU:HD13	1.96	0.47
1:A:271:PHE:CE2	1:A:291:LEU:HB2	2.50	0.47
1:A:172:PHE:O	1:A:176:ARG:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:501:NCT:HC82	2:D:502:HEM:NC	2.30	0.47
1:B:73:LEU:HB3	1:B:222:MET:HG2	1.97	0.47
1:D:400[B]:ARG:NH1	1:D:408:PRO:O	2.48	0.47
1:A:152:GLU:OE2	1:A:190:ARG:NE	2.48	0.47
1:C:187:PHE:HZ	1:C:248:ILE:HD13	1.79	0.46
1:C:314:PHE:HA	1:C:317:LEU:HD12	1.95	0.46
1:D:328:HIS:O	1:D:329:GLU:C	2.59	0.46
1:A:458:GLN:O	1:A:494:ARG:NH1	2.48	0.46
1:C:302:GLY:CA	2:C:500:HEM:HMC2	2.39	0.46
1:C:326:LYS:HB3	1:C:351:TYR:CE2	2.50	0.46
1:B:146:GLU:OE1	1:B:342:LYS:HB2	2.16	0.46
1:B:168:ILE:HD11	1:B:491:PHE:HE1	1.81	0.46
1:A:161:ARG:CZ	1:C:420:LYS:HD2	2.46	0.46
1:B:271:PHE:CB	1:B:291:LEU:HD13	2.46	0.46
1:D:318:MET:SD	1:D:489:MET:HE3	2.56	0.46
1:C:430:VAL:N	1:C:431:PRO:CD	2.79	0.45
1:A:40:LEU:HD23	1:A:40:LEU:HA	1.85	0.45
1:B:213:SER:O	1:B:477:HIS:HB3	2.17	0.45
1:C:271:PHE:CE2	1:C:291:LEU:HB2	2.52	0.45
1:B:95:ALA:O	1:B:99:SER:HB3	2.17	0.45
1:C:353:GLU:HG2	1:C:423:PHE:CE2	2.51	0.45
1:B:324:GLU:HG3	1:B:457:MET:HE1	1.99	0.45
1:A:51:THR:CG2	1:A:222:MET:HE3	2.46	0.44
1:A:327:VAL:HG13	1:A:352:MET:CE	2.48	0.44
1:D:430:VAL:N	1:D:431:PRO:CD	2.80	0.44
1:A:101:ARG:HG2	1:A:118:PHE:HA	2.00	0.44
1:D:271:PHE:CD2	1:D:291:LEU:HB2	2.52	0.44
1:D:205:MET:HE2	1:D:300:ILE:CG1	2.48	0.44
1:B:343:PHE:O	1:B:346:ARG:CB	2.66	0.44
1:B:84:HIS:NE2	1:B:427:ASP:HB3	2.32	0.43
1:C:440:PHE:CZ	2:C:500:HEM:HMD1	2.53	0.43
1:D:172:PHE:CZ	1:D:206:LEU:HD22	2.53	0.43
1:D:457:MET:HE2	1:D:457:MET:HA	2.00	0.43
1:A:51:THR:O	1:A:215:SER:HA	2.18	0.43
1:B:343:PHE:O	1:B:346:ARG:HB2	2.18	0.43
1:D:365:VAL:O	1:D:481:ALA:HA	2.19	0.43
1:B:197:GLU:O	1:B:201:LEU:HG	2.19	0.43
1:A:194:LYS:HA	1:A:194:LYS:HD3	1.91	0.43
1:C:314:PHE:HD2	1:C:317:LEU:HD12	1.83	0.43
1:D:116:VAL:CG1	1:D:294:THR:HG23	2.49	0.43
1:B:88:ARG:NH2	1:B:427:ASP:O	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ARG:NH1	1:B:148:ARG:HG3	2.34	0.42
1:C:199:LEU:HD21	1:C:203:ARG:NH2	2.27	0.42
1:C:363:GLY:O	1:C:482:THR:HG21	2.20	0.42
1:D:201:LEU:HD22	1:D:244:LEU:HD23	2.00	0.42
1:D:219:LEU:HD12	1:D:219:LEU:HA	1.89	0.42
1:B:365:VAL:O	1:B:481:ALA:HA	2.19	0.42
1:B:348:LYS:C	1:B:350:PRO:HD2	2.45	0.42
1:D:35:PRO:O	1:D:69:PHE:HB2	2.20	0.42
1:D:418:ASN:CG	1:D:419:GLU:N	2.76	0.42
1:D:439:CYS:HB2	2:D:502:HEM:NA	2.33	0.42
1:B:465:SER:HB2	1:B:466:GLN:HG3	2.01	0.42
1:D:412:ASN:OD1	1:D:414:GLN:HB2	2.20	0.42
1:C:161:ARG:NH2	1:C:459:ASN:OD1	2.53	0.42
1:C:330:GLU:HG3	1:C:333:ARG:NH2	2.35	0.42
1:A:201:LEU:O	1:A:204:MET:HB2	2.20	0.41
1:D:305:THR:CG2	3:D:501:NCT:HC92	2.46	0.41
1:A:439:CYS:HB2	2:A:500:HEM:NA	2.35	0.41
1:D:180:ASN:HA	1:D:183:SER:HB2	2.02	0.41
1:D:353:GLU:HG2	1:D:423:PHE:CE2	2.55	0.41
1:A:374:VAL:HG22	1:A:389:THR:O	2.20	0.41
1:B:401:ASP:OD2	1:B:401:ASP:C	2.63	0.41
1:C:34:PRO:HA	1:C:383:PHE:CE2	2.55	0.41
1:D:73:LEU:HD12	1:D:78:VAL:HG21	2.02	0.41
1:D:315:LEU:HB2	1:D:487:TYR:CE2	2.55	0.41
1:D:340:GLN:HA	1:D:341:PRO:HD2	1.94	0.41
1:D:313:GLY:HA3	1:D:359:ILE:HD13	2.02	0.41
1:D:315:LEU:O	1:D:315:LEU:HG	2.20	0.41
1:A:143:ARG:O	1:A:144:GLY:C	2.62	0.41
1:D:420:LYS:HB2	1:D:422:GLN:HG3	2.03	0.41
1:C:205:MET:HE1	1:C:299:PHE:CE2	2.56	0.41
1:C:356:ILE:CD1	1:C:450:PHE:HA	2.51	0.41
1:A:200:SER:O	1:A:204:MET:HG3	2.21	0.40
1:A:424:LYS:HB3	1:A:424:LYS:HE2	1.66	0.40
1:C:209:PHE:HZ	3:C:501:NCT:H102	1.86	0.40
1:C:275:MET:HG2	1:C:286:PHE:O	2.21	0.40
1:B:145:ILE:HD12	1:B:145:ILE:HA	1.86	0.40
1:C:271:PHE:HB3	1:C:291:LEU:HD13	2.02	0.40
1:C:273:ILE:O	1:C:274:ARG:C	2.63	0.40
1:D:182:ILE:O	1:D:185:ILE:HB	2.21	0.40
1:D:323:VAL:O	1:D:327:VAL:HG23	2.21	0.40
1:A:433:SER:O	1:A:434:ILE:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:ARG:HD3	4:A:630:HOH:O	2.21	0.40
1:B:48:GLN:H	1:B:48:GLN:HG2	1.55	0.40
1:C:32:LYS:O	1:C:33:LEU:C	2.64	0.40
1:D:463:LYS:HD3	1:D:463:LYS:HA	1.78	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	466/476 (98%)	434 (93%)	30 (6%)	2 (0%)	30	38
1	B	464/476 (98%)	441 (95%)	23 (5%)	0	100	100
1	C	463/476 (97%)	431 (93%)	30 (6%)	2 (0%)	30	38
1	D	465/476 (98%)	433 (93%)	31 (7%)	1 (0%)	43	55
All	All	1858/1904 (98%)	1739 (94%)	114 (6%)	5 (0%)	36	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	GLY
1	D	162	GLY
1	A	195	ASP
1	C	33	LEU
1	C	181	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	415/422 (98%)	396 (95%)	19 (5%)	24	36
1	B	413/422 (98%)	398 (96%)	15 (4%)	31	47
1	C	412/422 (98%)	397 (96%)	15 (4%)	31	47
1	D	414/422 (98%)	385 (93%)	29 (7%)	14	19
All	All	1654/1688 (98%)	1576 (95%)	78 (5%)	24	35

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LYS
1	A	32	LYS
1	A	64[A]	ARG
1	A	64[B]	ARG
1	A	103	GLU
1	A	135	LEU
1	A	145	ILE
1	A	168	ILE
1	A	194	LYS
1	A	253	GLU
1	A	262	ASN
1	A	279	GLU
1	A	284	THR
1	A	305	THR
1	A	374	VAL
1	A	375	LYS
1	A	376	LYS
1	A	425	LYS
1	A	469	LYS
1	B	32	LYS
1	B	48	GLN
1	B	135	LEU
1	B	145	ILE
1	B	167	ASN
1	B	236	GLN
1	B	307	SER
1	B	312	TYR
1	B	326	LYS
1	B	337	LYS
1	B	379[A]	LYS

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Mol	Chain	Res	Type
1	B	379[B]	LYS
1	B	420	LYS
1	B	464	SER
1	B	467	SER
1	C	32	LYS
1	C	40	LEU
1	C	122	GLU
1	C	167	ASN
1	C	168	ILE
1	C	236	GLN
1	C	274	ARG
1	C	305	THR
1	C	353	GLU
1	C	370	LEU
1	C	376	LYS
1	C	420	LYS
1	C	434	ILE
1	C	457	MET
1	C	463	LYS
1	D	60	LYS
1	D	75	PRO
1	D	125	LYS
1	D	129	ARG
1	D	135	LEU
1	D	168	ILE
1	D	236	GLN
1	D	250	LYS
1	D	253	GLU
1	D	259	LEU
1	D	263	SER
1	D	276	GLN
1	D	305	THR
1	D	339	ARG
1	D	344	GLU
1	D	346	ARG
1	D	353	GLU
1	D	355	VAL
1	D	370	LEU
1	D	407	ASN
1	D	419	GLU
1	D	434	ILE
1	D	453	PHE

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Mol	Chain	Res	Type
1	D	457	MET
1	D	461	ARG
1	D	463	LYS
1	D	465	SER
1	D	469	LYS
1	D	478	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	ASN
1	A	229	HIS
1	A	235	GLN
1	A	256	GLN
1	A	297	ASN
1	A	409	GLN
1	B	72	HIS
1	B	150	GLN
1	B	409	GLN
1	C	256	GLN
1	C	297	ASN
1	C	360	GLN
1	C	407	ASN
1	C	409	GLN
1	D	56	ASN
1	D	297	ASN
1	D	414	GLN
1	D	422	GLN
1	D	458	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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
2	HEM	D	502	1	50,50,50	2.12	12 (24%)	67,82,82	1.65	12 (17%)
2	HEM	C	500	1	50,50,50	2.18	11 (22%)	67,82,82	1.54	8 (11%)
3	NCT	B	501	-	13,13,13	1.07	1 (7%)	17,17,17	2.24	5 (29%)
2	HEM	B	500	1	50,50,50	2.38	15 (30%)	67,82,82	1.69	16 (23%)
2	HEM	A	500	1	50,50,50	2.35	14 (28%)	67,82,82	1.88	19 (28%)
3	NCT	D	501	-	13,13,13	0.64	0	17,17,17	2.39	5 (29%)
3	NCT	A	501	-	13,13,13	1.14	1 (7%)	17,17,17	2.62	9 (52%)
3	NCT	C	501	-	13,13,13	0.76	0	17,17,17	2.16	7 (41%)

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	D	502	1	-	4/14/54/54	-
2	HEM	C	500	1	-	6/14/54/54	-
3	NCT	B	501	-	-	0/4/14/14	0/2/2/2
2	HEM	B	500	1	-	3/14/54/54	-
2	HEM	A	500	1	-	6/14/54/54	-
3	NCT	D	501	-	-	1/4/14/14	0/2/2/2
3	NCT	A	501	-	-	0/4/14/14	0/2/2/2
3	NCT	C	501	-	-	1/4/14/14	0/2/2/2

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	502	HEM	C3D-C2D	8.28	1.54	1.36
2	C	500	HEM	FE-ND	8.19	2.20	1.94
2	A	500	HEM	C3D-C2D	8.02	1.54	1.36
2	B	500	HEM	C3D-C2D	7.43	1.52	1.36
2	B	500	HEM	FE-ND	7.17	2.17	1.94
2	C	500	HEM	C3D-C2D	7.08	1.52	1.36
2	D	502	HEM	FE-ND	6.33	2.14	1.94
2	A	500	HEM	FE-ND	5.73	2.12	1.94
2	A	500	HEM	FE-NA	5.68	2.13	1.95
2	B	500	HEM	FE-NC	5.28	2.12	1.95
2	A	500	HEM	FE-NC	5.10	2.12	1.95
2	C	500	HEM	FE-NB	4.90	2.10	1.94
2	D	502	HEM	FE-NC	4.20	2.09	1.95
2	B	500	HEM	FE-NB	4.15	2.07	1.94
2	A	500	HEM	CAB-C3B	3.96	1.58	1.47
2	B	500	HEM	FE-NA	3.90	2.08	1.95
2	C	500	HEM	CAC-C3C	3.90	1.57	1.47
2	B	500	HEM	CMB-C2B	3.84	1.58	1.50
2	A	500	HEM	FE-NB	3.57	2.05	1.94
2	D	502	HEM	FE-NB	3.54	2.05	1.94
2	D	502	HEM	CMC-C2C	3.47	1.57	1.50
3	B	501	NCT	C2-C6	-3.36	1.46	1.51
3	A	501	NCT	C2-C6	-3.29	1.46	1.51
2	D	502	HEM	CAB-C3B	3.28	1.56	1.47
2	C	500	HEM	CAB-C3B	3.28	1.56	1.47
2	B	500	HEM	CMC-C2C	3.13	1.57	1.50
2	B	500	HEM	CAC-C3C	3.12	1.55	1.47
2	A	500	HEM	C1C-NC	-3.10	1.33	1.39
2	B	500	HEM	C1C-NC	-3.02	1.33	1.39
2	B	500	HEM	CAB-C3B	2.98	1.55	1.47
2	A	500	HEM	CMB-C2B	2.90	1.56	1.50
2	A	500	HEM	C4B-NB	-2.80	1.33	1.38
2	D	502	HEM	CMB-C2B	2.72	1.56	1.50
2	C	500	HEM	CMD-C2D	2.69	1.56	1.50
2	C	500	HEM	FE-NC	2.63	2.03	1.95
2	B	500	HEM	C1B-NB	-2.57	1.35	1.40
2	B	500	HEM	CAA-C2A	2.54	1.57	1.51
2	D	502	HEM	C4D-ND	-2.51	1.35	1.40
2	B	500	HEM	C4B-NB	-2.50	1.33	1.38
2	C	500	HEM	C1B-NB	-2.49	1.35	1.40
2	D	502	HEM	FE-NA	2.39	2.03	1.95
2	D	502	HEM	CAC-C3C	2.30	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	O2D-CGD	-2.30	1.23	1.30
2	C	500	HEM	CMB-C2B	2.26	1.55	1.50
2	D	502	HEM	CMD-C2D	2.24	1.55	1.50
2	C	500	HEM	C2A-C3A	-2.20	1.33	1.38
2	A	500	HEM	C3C-C4C	-2.16	1.42	1.46
2	A	500	HEM	O2A-CGA	-2.15	1.23	1.30
2	A	500	HEM	CAC-C3C	2.14	1.53	1.47
2	A	500	HEM	C1A-NA	-2.12	1.35	1.39
2	D	502	HEM	CAA-C2A	2.05	1.56	1.51
2	C	500	HEM	C4D-ND	-2.05	1.36	1.40
2	B	500	HEM	C4A-NA	-2.04	1.35	1.39
2	B	500	HEM	C4C-NC	-2.00	1.35	1.39

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	502	HEM	C4D-ND-C1D	7.53	114.12	105.21
2	A	500	HEM	C4D-ND-C1D	6.89	113.36	105.21
2	B	500	HEM	C4D-ND-C1D	6.56	112.98	105.21
2	C	500	HEM	C4D-ND-C1D	6.12	112.46	105.21
3	D	501	NCT	C10-N2-C6	5.14	128.09	112.78
2	A	500	HEM	C3B-C4B-NB	-5.09	105.81	109.47
3	A	501	NCT	C3-C2-C1	4.91	121.95	116.89
3	A	501	NCT	C10-N2-C6	4.75	126.94	112.78
2	A	500	HEM	C1B-NB-C4B	4.29	110.28	105.21
3	C	501	NCT	C10-N2-C6	4.23	125.38	112.78
3	B	501	NCT	C3-C2-C1	4.19	121.21	116.89
3	D	501	NCT	C2-C6-N2	4.09	122.93	112.17
3	D	501	NCT	C7-C6-N2	-4.04	91.48	102.55
3	B	501	NCT	C10-N2-C9	3.99	124.69	112.68
3	B	501	NCT	C4-C3-C2	-3.88	116.00	120.65
3	A	501	NCT	C10-N2-C9	3.69	123.78	112.68
3	A	501	NCT	C2-C1-N1	-3.41	118.73	124.05
2	C	500	HEM	C1B-NB-C4B	3.40	109.23	105.21
3	C	501	NCT	C8-C9-N2	-3.40	93.90	103.56
2	B	500	HEM	O1A-CGA-CBA	-3.35	112.48	123.09
3	C	501	NCT	C3-C2-C1	3.34	120.33	116.89
2	C	500	HEM	CHB-C4A-NA	3.30	129.85	123.86
3	D	501	NCT	C10-N2-C9	3.18	122.24	112.68
2	A	500	HEM	CHC-C4B-NB	3.09	127.75	124.42
3	B	501	NCT	C9-N2-C6	3.09	113.42	104.28
3	A	501	NCT	C1-C2-C6	-3.06	115.17	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	NCT	C10-N2-C9	3.06	121.88	112.68
3	B	501	NCT	C10-N2-C6	3.05	121.88	112.78
2	D	502	HEM	CHD-C1D-ND	3.02	127.67	124.42
2	B	500	HEM	CMB-C2B-C1B	3.01	129.74	125.03
2	D	502	HEM	C4C-C3C-C2C	2.95	109.38	106.81
2	B	500	HEM	O2A-CGA-CBA	2.93	123.27	114.00
2	B	500	HEM	C1C-CHC-C4B	2.89	132.16	126.02
2	B	500	HEM	C3B-C2B-C1B	-2.86	104.26	106.41
3	C	501	NCT	C9-N2-C6	2.84	112.69	104.28
2	A	500	HEM	CMA-C3A-C4A	-2.83	121.10	125.42
2	A	500	HEM	C4B-C3B-C2B	2.82	109.88	107.28
2	D	502	HEM	CBC-CAC-C3C	-2.82	113.44	127.53
2	A	500	HEM	C2A-C1A-NA	-2.82	107.03	110.15
3	C	501	NCT	C2-C1-N1	-2.81	119.67	124.05
3	D	501	NCT	C5-N1-C1	2.77	121.71	116.85
3	A	501	NCT	C4-C3-C2	-2.76	117.34	120.65
2	C	500	HEM	C3B-C4B-NB	-2.72	107.51	109.47
2	B	500	HEM	C4C-NC-C1C	2.72	110.25	105.82
2	A	500	HEM	C4A-NA-C1A	2.70	110.22	105.82
2	A	500	HEM	C4C-NC-C1C	2.70	110.22	105.82
2	C	500	HEM	CAD-C3D-C4D	2.68	129.37	124.70
2	B	500	HEM	C4A-C3A-C2A	2.62	109.81	106.82
2	C	500	HEM	C4A-C3A-C2A	2.61	109.81	106.82
2	A	500	HEM	C3C-C2C-C1C	2.61	109.51	107.05
3	A	501	NCT	C5-N1-C1	2.60	121.41	116.85
2	D	502	HEM	C1B-NB-C4B	2.60	108.29	105.21
2	B	500	HEM	C4A-NA-C1A	2.58	110.03	105.82
2	D	502	HEM	CHD-C4C-C3C	2.47	129.37	125.21
2	B	500	HEM	C1A-CHA-C4D	2.44	131.99	126.25
2	B	500	HEM	C1B-NB-C4B	2.44	108.10	105.21
2	D	502	HEM	C2A-C1A-NA	-2.44	107.45	110.15
2	D	502	HEM	CHC-C1C-NC	2.44	127.11	124.45
2	B	500	HEM	C2A-C1A-NA	-2.43	107.45	110.15
2	D	502	HEM	C2D-C1D-ND	-2.43	107.09	109.90
3	C	501	NCT	C5-N1-C1	2.42	121.09	116.85
2	D	502	HEM	O2A-CGA-CBA	2.37	121.48	114.00
2	A	500	HEM	CHD-C1D-ND	2.35	126.95	124.42
2	A	500	HEM	CHA-C4D-ND	2.31	127.23	124.37
2	D	502	HEM	C3D-C4D-ND	-2.27	107.68	110.17
2	A	500	HEM	CBA-CAA-C2A	-2.27	106.25	112.53
3	A	501	NCT	C7-C6-C2	2.26	118.20	113.69
2	A	500	HEM	C3A-C4A-NA	-2.26	106.53	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	HEM	CAD-CBD-CGD	-2.25	107.71	113.67
3	A	501	NCT	C7-C6-N2	-2.23	96.43	102.55
2	B	500	HEM	C3A-C4A-NA	-2.23	106.57	110.14
2	A	500	HEM	C2D-C1D-ND	-2.23	107.33	109.90
2	A	500	HEM	CMB-C2B-C1B	2.22	128.51	125.03
2	B	500	HEM	C4B-C3B-C2B	2.22	109.32	107.28
2	C	500	HEM	C3B-C2B-C1B	2.19	108.06	106.41
2	A	500	HEM	C3D-C4D-ND	-2.11	107.86	110.17
2	D	502	HEM	C1D-C2D-C3D	-2.09	104.78	106.98
2	A	500	HEM	CMA-C3A-C2A	2.08	130.03	125.62
2	B	500	HEM	CHB-C1B-NB	-2.07	121.80	124.37
2	C	500	HEM	C3A-C4A-NA	-2.05	106.85	110.14
2	A	500	HEM	C1C-CHC-C4B	2.00	130.28	126.02

There are no chirality outliers.

All (21) torsion outliers are listed below:

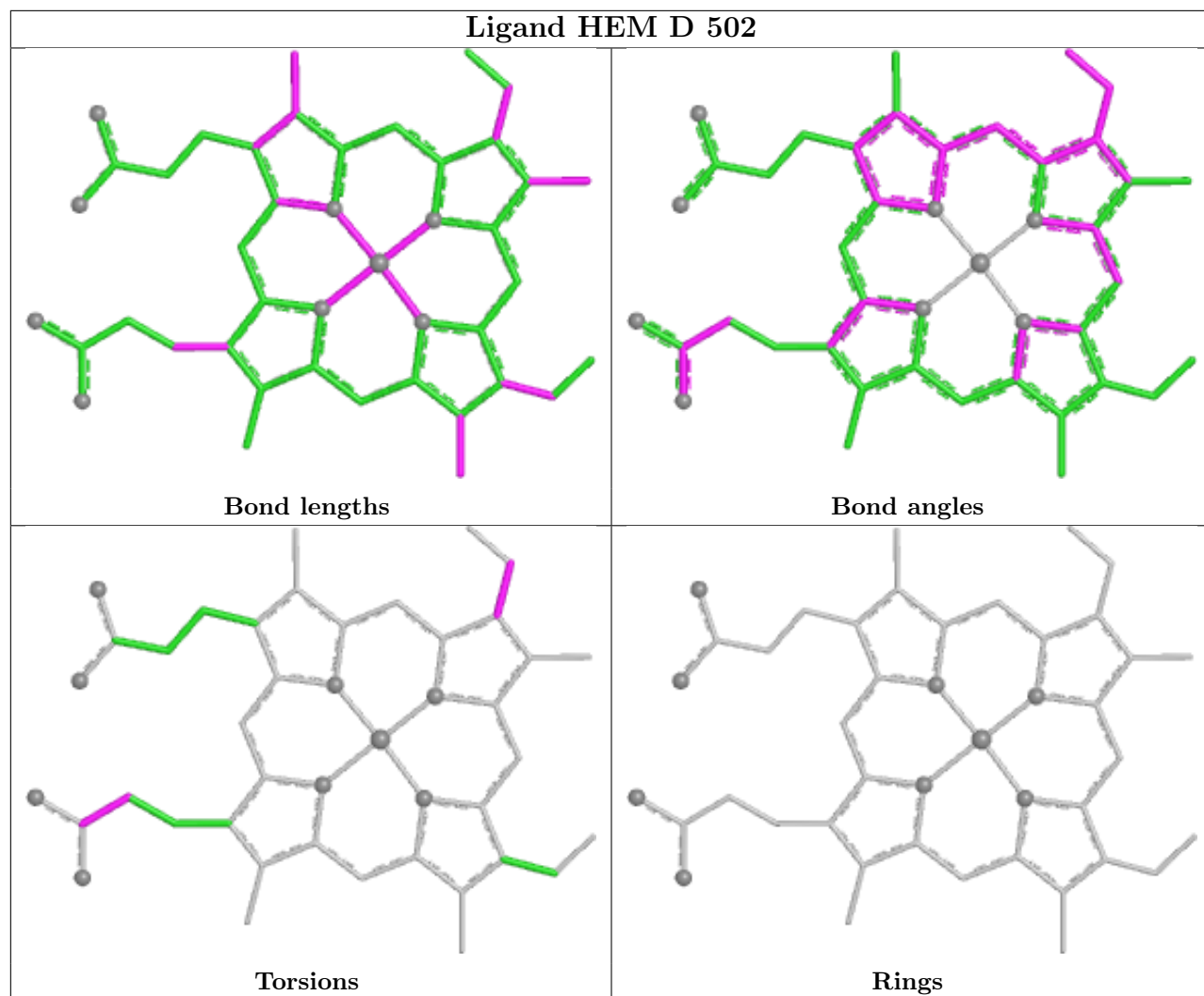
Mol	Chain	Res	Type	Atoms
2	A	500	HEM	C2C-C3C-CAC-CBC
2	A	500	HEM	C4C-C3C-CAC-CBC
2	B	500	HEM	C2C-C3C-CAC-CBC
2	B	500	HEM	C4C-C3C-CAC-CBC
2	C	500	HEM	C2C-C3C-CAC-CBC
2	C	500	HEM	C4C-C3C-CAC-CBC
2	D	502	HEM	C2C-C3C-CAC-CBC
2	D	502	HEM	C4C-C3C-CAC-CBC
3	D	501	NCT	C1-C2-C6-N2
3	C	501	NCT	C1-C2-C6-C7
2	C	500	HEM	CAA-CBA-CGA-O1A
2	C	500	HEM	CAA-CBA-CGA-O2A
2	A	500	HEM	CAA-CBA-CGA-O1A
2	C	500	HEM	CAD-CBD-CGD-O1D
2	A	500	HEM	CAD-CBD-CGD-O1D
2	A	500	HEM	CAA-CBA-CGA-O2A
2	C	500	HEM	CAD-CBD-CGD-O2D
2	D	502	HEM	CAA-CBA-CGA-O1A
2	A	500	HEM	CAD-CBD-CGD-O2D
2	B	500	HEM	CAA-CBA-CGA-O2A
2	D	502	HEM	CAA-CBA-CGA-O2A

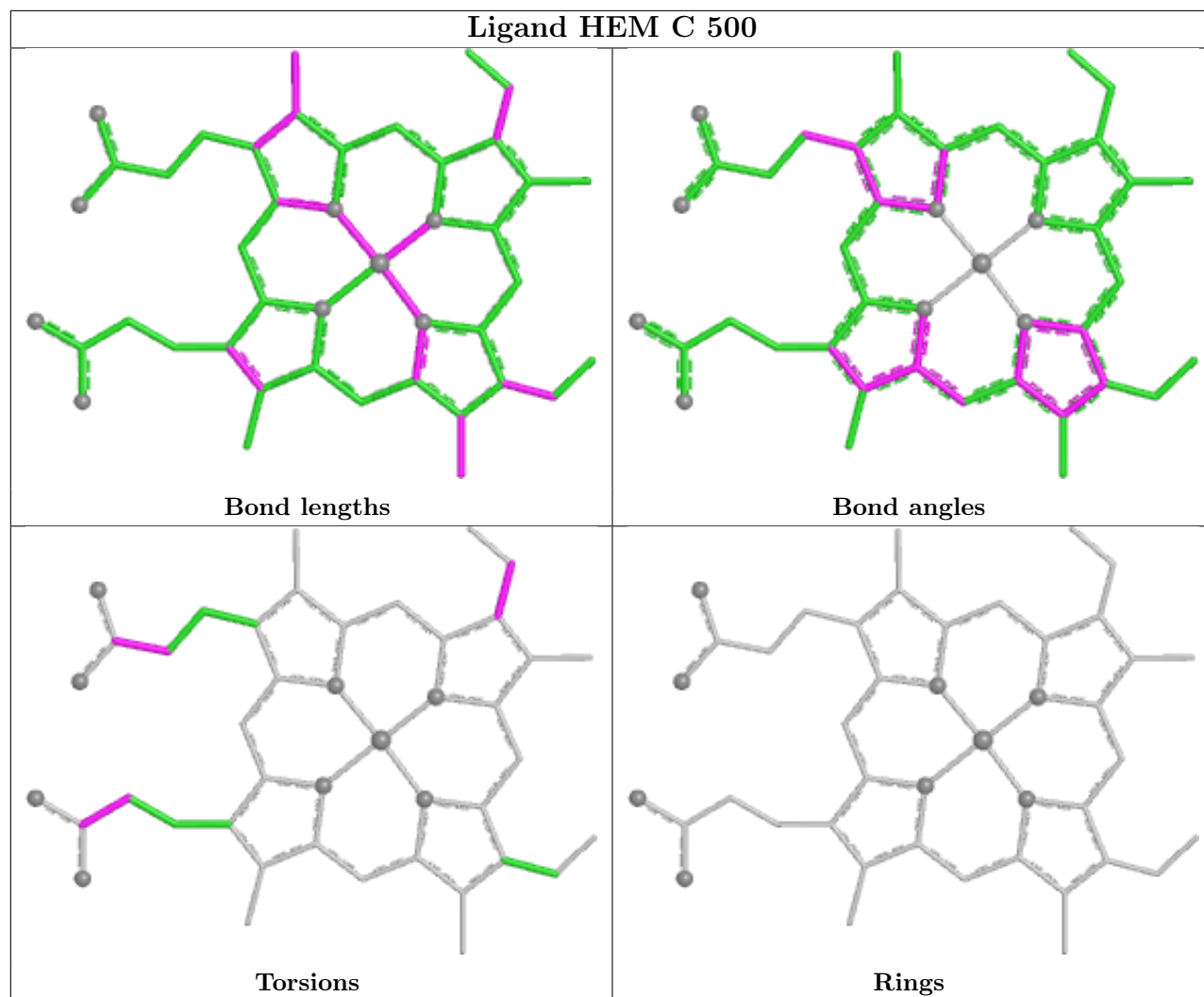
There are no ring outliers.

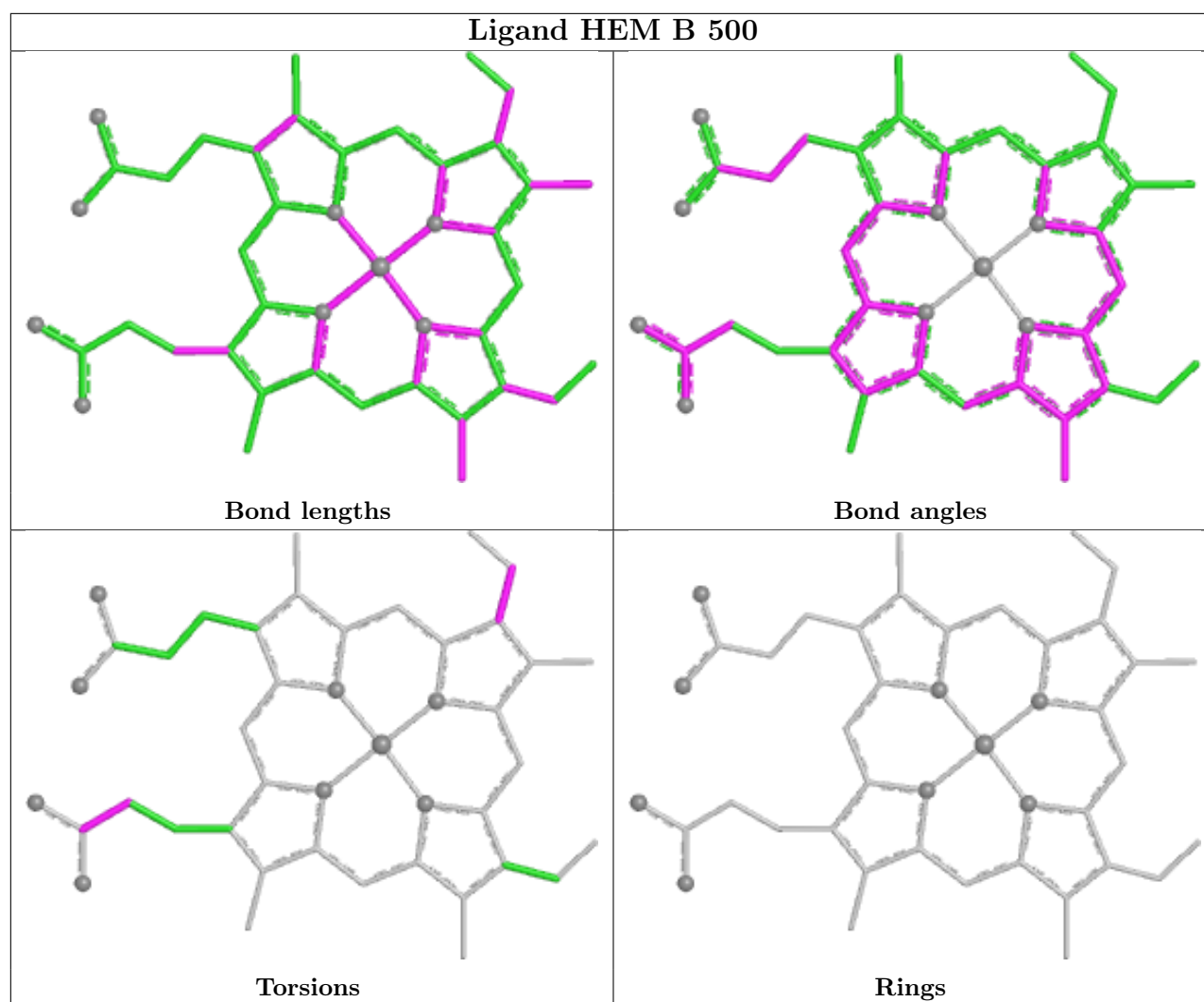
8 monomers are involved in 41 short contacts:

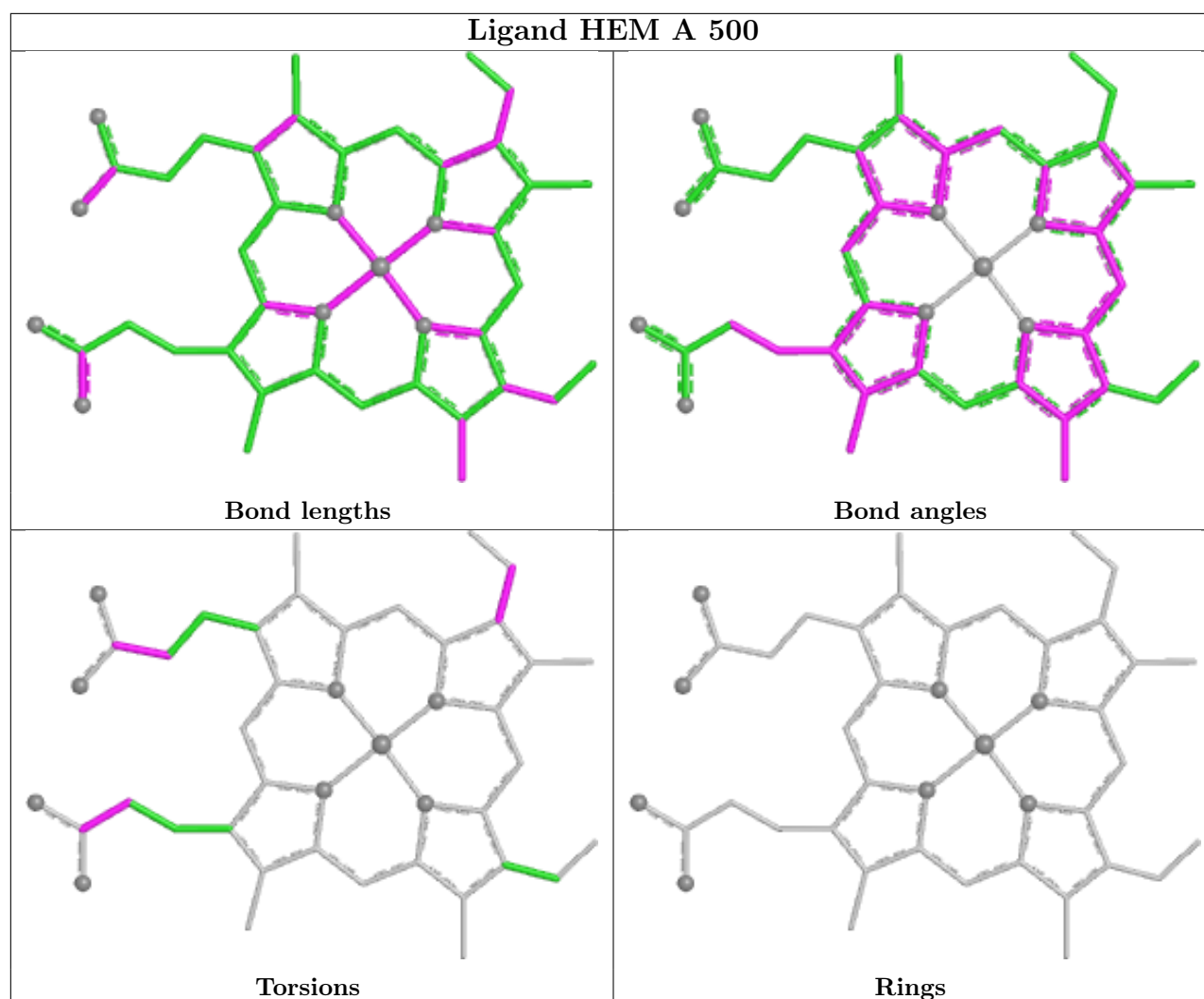
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	502	HEM	6	0
2	C	500	HEM	8	0
3	B	501	NCT	6	0
2	B	500	HEM	9	0
2	A	500	HEM	4	0
3	D	501	NCT	6	0
3	A	501	NCT	3	0
3	C	501	NCT	6	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	465/476 (97%)	-0.14	4 (0%)	81 82	16, 33, 54, 65	3 (0%)
1	B	464/476 (97%)	0.04	3 (0%)	85 86	22, 40, 58, 70	2 (0%)
1	C	464/476 (97%)	0.26	5 (1%)	78 79	20, 44, 60, 67	1 (0%)
1	D	464/476 (97%)	0.29	16 (3%)	48 50	17, 41, 65, 74	3 (0%)
All	All	1857/1904 (97%)	0.11	28 (1%)	72 73	16, 40, 61, 74	9 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	168	ILE	4.2
1	A	189	ASP	4.0
1	C	364	ASP	3.5
1	B	108	ASP	3.4
1	D	337	LYS	3.4
1	D	468	PRO	3.1
1	C	382	ASP	3.0
1	D	382	ASP	2.9
1	C	43	ILE	2.7
1	D	453	PHE	2.7
1	D	494	ARG	2.6
1	A	30	LYS	2.6
1	D	166	ALA	2.5
1	B	31	GLY	2.5
1	A	194	LYS	2.4
1	D	493	PRO	2.4
1	B	109	TRP	2.4
1	A	257	ARG	2.3
1	D	492	LEU	2.3
1	C	321	PRO	2.2
1	C	129	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	465	SER	2.2
1	D	167	ASN	2.1
1	D	163	THR	2.1
1	D	456	VAL	2.1
1	D	491	PHE	2.1
1	D	457	MET	2.0
1	D	467	SER	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](#)

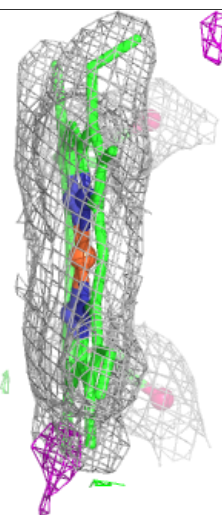
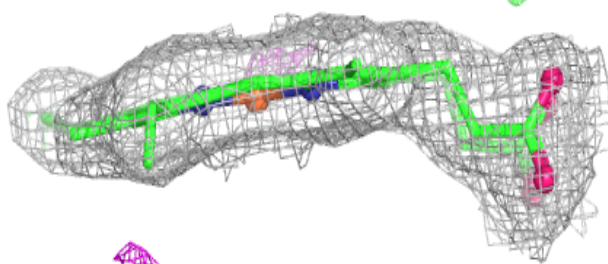
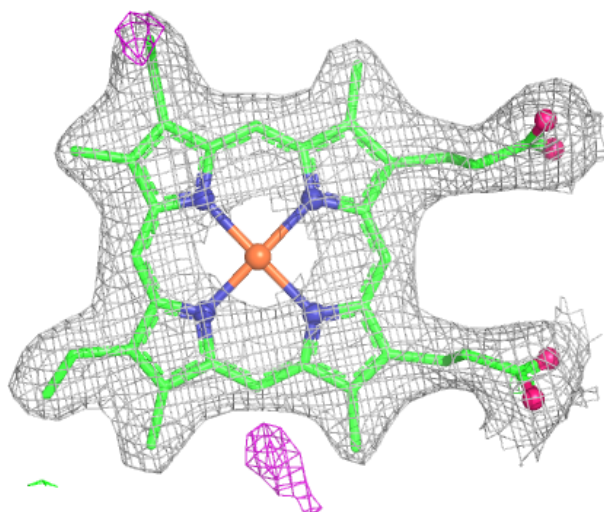
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NCT	A	501	12/12	0.92	0.12	45,48,49,49	0
3	NCT	C	501	12/12	0.92	0.14	52,57,63,63	0
3	NCT	D	501	12/12	0.92	0.17	60,64,66,66	0
3	NCT	B	501	12/12	0.95	0.11	51,53,57,57	0
2	HEM	A	500	43/43	0.98	0.06	19,26,30,31	0
2	HEM	B	500	43/43	0.98	0.06	24,31,35,41	0
2	HEM	C	500	43/43	0.98	0.07	31,38,42,45	0
2	HEM	D	502	43/43	0.98	0.07	24,33,39,47	0

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

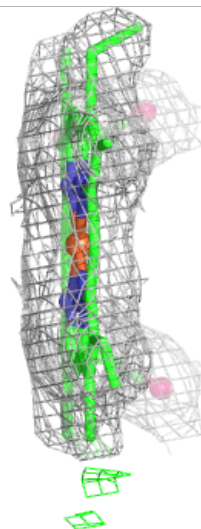
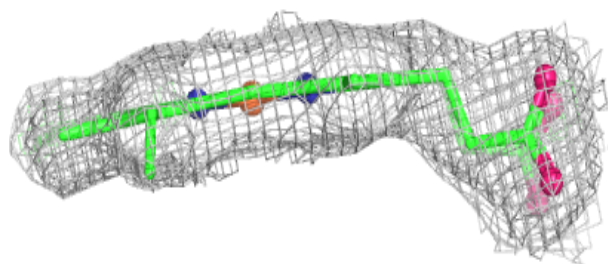
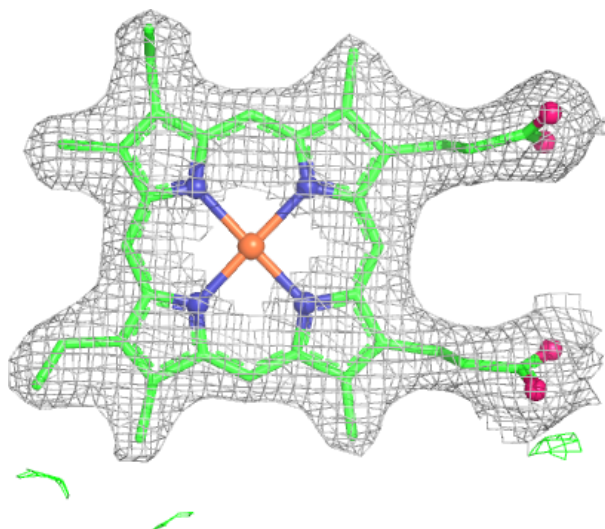
Electron density around HEM A 500:

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



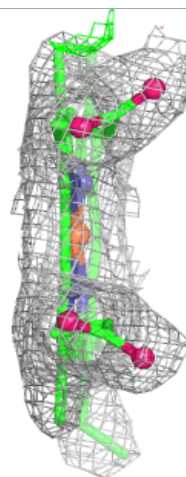
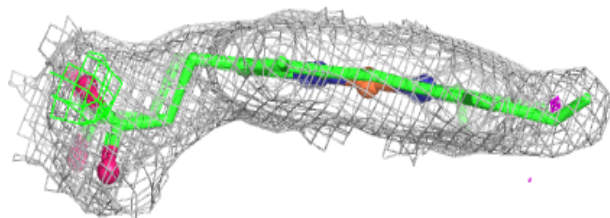
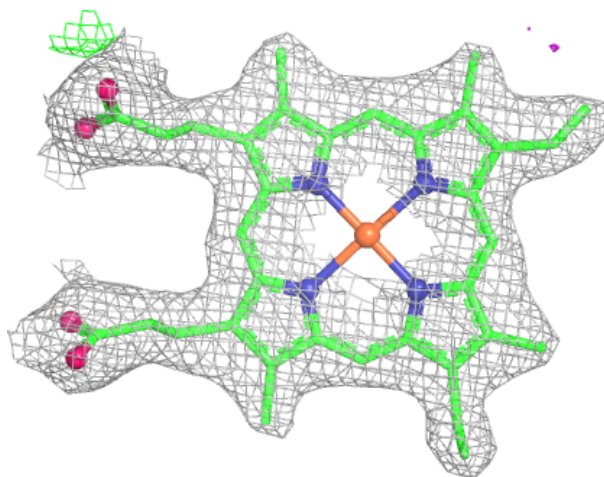
Electron density around HEM B 500:

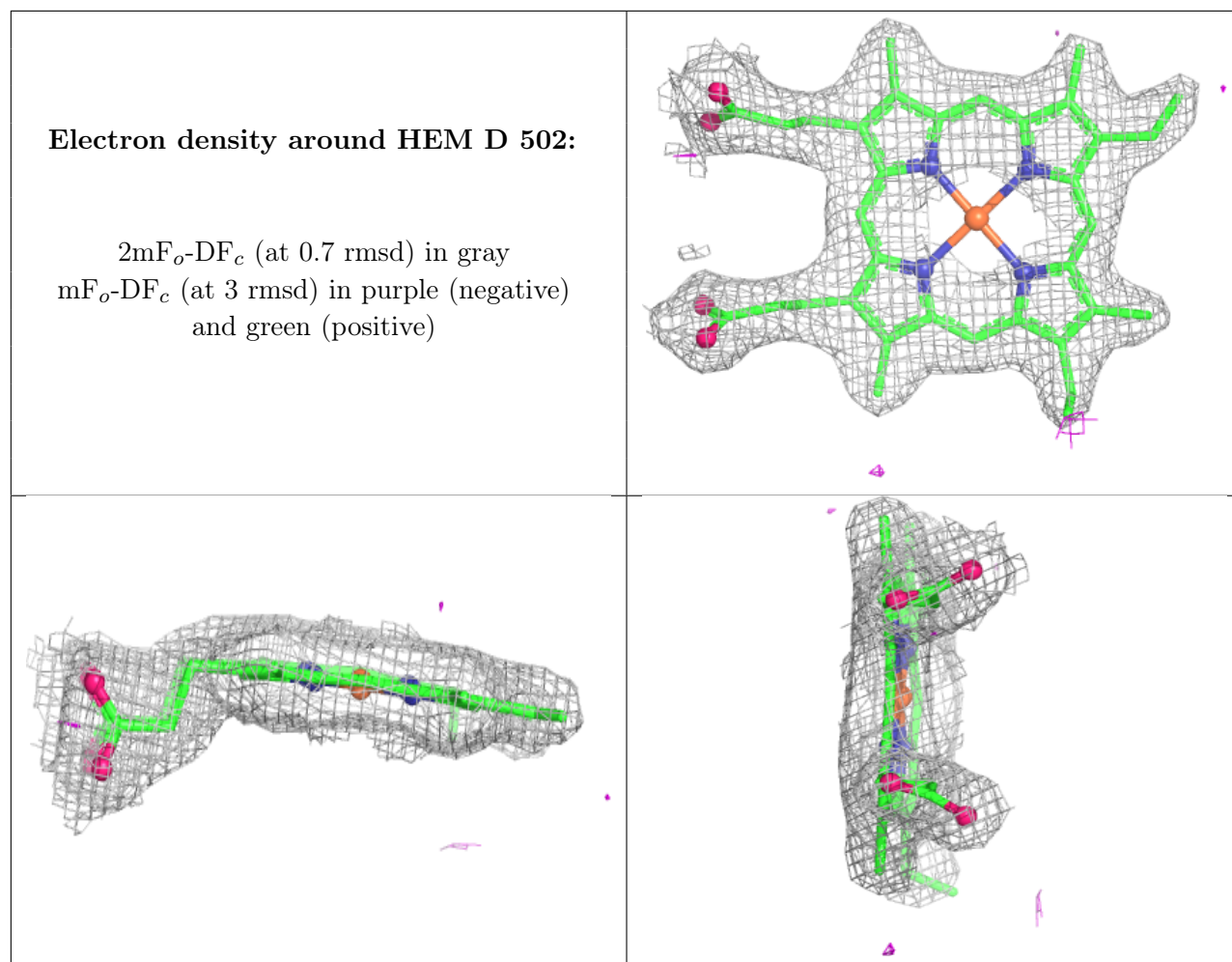
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 500:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.