



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 02:55 PM UTC

PDB ID : 3NC6 / pdb_00003nc6
Title : CYP134A1 1-phenylimidazole bound structure
Authors : Cryle, M.J.; Schlichting, I.
Deposited on : 2010-06-04
Resolution : 3.10 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

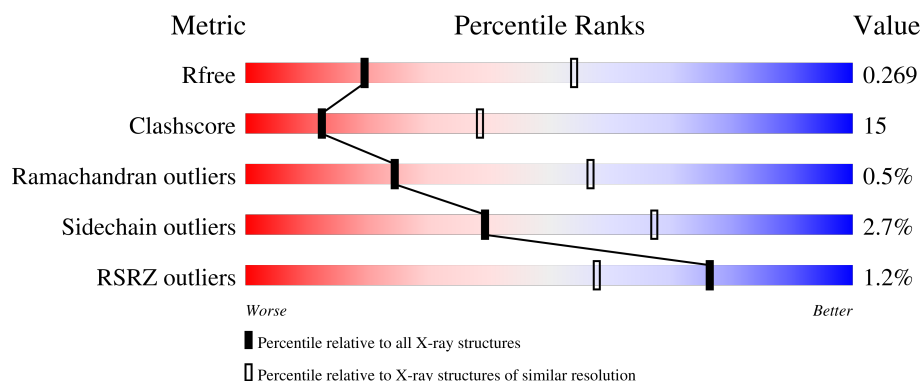
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	441	 59% 23% 15%
1	B	441	 66% 20% 12%

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
4	MG	A	408	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6150 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 cypX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	1	0
			2968	1885	511	558	14			
1	B	389	Total	C	N	O	S	0	0	0
			3068	1943	527	582	16			

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	expression tag	UNP O34926
A	-34	GLY	-	expression tag	UNP O34926
A	-33	SER	-	expression tag	UNP O34926
A	-32	SER	-	expression tag	UNP O34926
A	-31	HIS	-	expression tag	UNP O34926
A	-30	HIS	-	expression tag	UNP O34926
A	-29	HIS	-	expression tag	UNP O34926
A	-28	HIS	-	expression tag	UNP O34926
A	-27	HIS	-	expression tag	UNP O34926
A	-26	HIS	-	expression tag	UNP O34926
A	-25	SER	-	expression tag	UNP O34926
A	-24	SER	-	expression tag	UNP O34926
A	-23	GLY	-	expression tag	UNP O34926
A	-22	LEU	-	expression tag	UNP O34926
A	-21	VAL	-	expression tag	UNP O34926
A	-20	PRO	-	expression tag	UNP O34926
A	-19	ARG	-	expression tag	UNP O34926
A	-18	GLY	-	expression tag	UNP O34926
A	-17	SER	-	expression tag	UNP O34926
A	-16	HIS	-	expression tag	UNP O34926
A	-15	MET	-	expression tag	UNP O34926
A	-14	ALA	-	expression tag	UNP O34926
A	-13	SER	-	expression tag	UNP O34926
A	-12	MET	-	expression tag	UNP O34926
A	-11	THR	-	expression tag	UNP O34926

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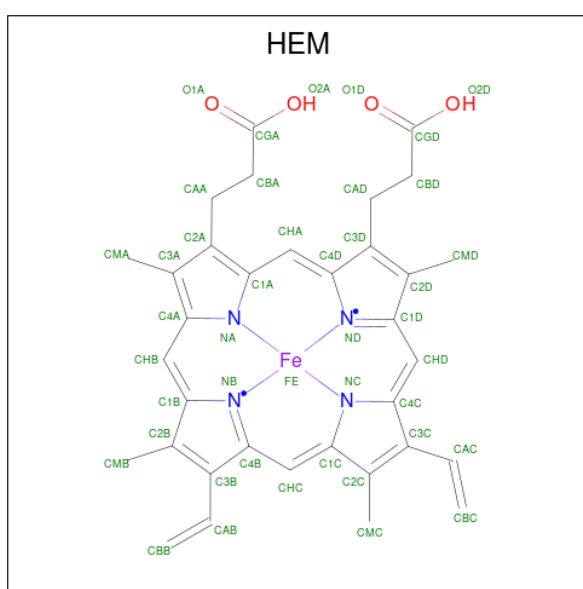
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLY	-	expression tag	UNP O34926
A	-9	GLY	-	expression tag	UNP O34926
A	-8	GLN	-	expression tag	UNP O34926
A	-7	GLN	-	expression tag	UNP O34926
A	-6	MET	-	expression tag	UNP O34926
A	-5	GLY	-	expression tag	UNP O34926
A	-4	ARG	-	expression tag	UNP O34926
A	-3	GLY	-	expression tag	UNP O34926
A	-2	SER	-	expression tag	UNP O34926
A	-1	GLU	-	expression tag	UNP O34926
A	0	PHE	-	expression tag	UNP O34926
A	356	THR	ALA	engineered mutation	UNP O34926
B	-35	MET	-	expression tag	UNP O34926
B	-34	GLY	-	expression tag	UNP O34926
B	-33	SER	-	expression tag	UNP O34926
B	-32	SER	-	expression tag	UNP O34926
B	-31	HIS	-	expression tag	UNP O34926
B	-30	HIS	-	expression tag	UNP O34926
B	-29	HIS	-	expression tag	UNP O34926
B	-28	HIS	-	expression tag	UNP O34926
B	-27	HIS	-	expression tag	UNP O34926
B	-26	HIS	-	expression tag	UNP O34926
B	-25	SER	-	expression tag	UNP O34926
B	-24	SER	-	expression tag	UNP O34926
B	-23	GLY	-	expression tag	UNP O34926
B	-22	LEU	-	expression tag	UNP O34926
B	-21	VAL	-	expression tag	UNP O34926
B	-20	PRO	-	expression tag	UNP O34926
B	-19	ARG	-	expression tag	UNP O34926
B	-18	GLY	-	expression tag	UNP O34926
B	-17	SER	-	expression tag	UNP O34926
B	-16	HIS	-	expression tag	UNP O34926
B	-15	MET	-	expression tag	UNP O34926
B	-14	ALA	-	expression tag	UNP O34926
B	-13	SER	-	expression tag	UNP O34926
B	-12	MET	-	expression tag	UNP O34926
B	-11	THR	-	expression tag	UNP O34926
B	-10	GLY	-	expression tag	UNP O34926
B	-9	GLY	-	expression tag	UNP O34926
B	-8	GLN	-	expression tag	UNP O34926
B	-7	GLN	-	expression tag	UNP O34926
B	-6	MET	-	expression tag	UNP O34926

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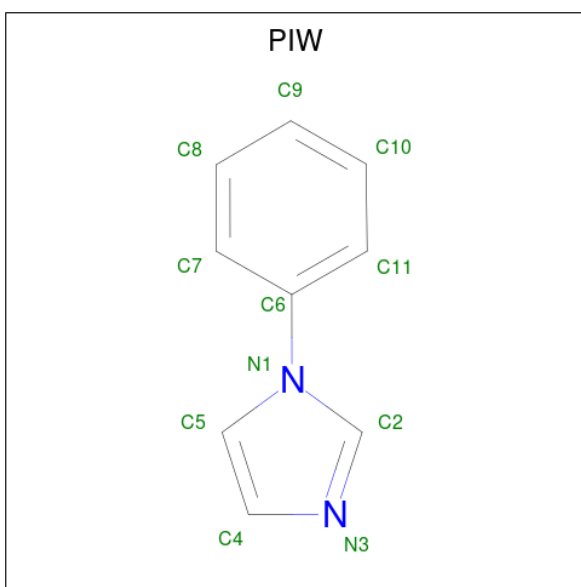
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLY	-	expression tag	UNP O34926
B	-4	ARG	-	expression tag	UNP O34926
B	-3	GLY	-	expression tag	UNP O34926
B	-2	SER	-	expression tag	UNP O34926
B	-1	GLU	-	expression tag	UNP O34926
B	0	PHE	-	expression tag	UNP O34926
B	356	THR	ALA	engineered mutation	UNP O34926

- 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	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 1-phenyl-1H-imidazole (CCD ID: PIW) (formula: $C_9H_8N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			11	9	2		
3	B	1	Total	C	N	0	0
			11	9	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

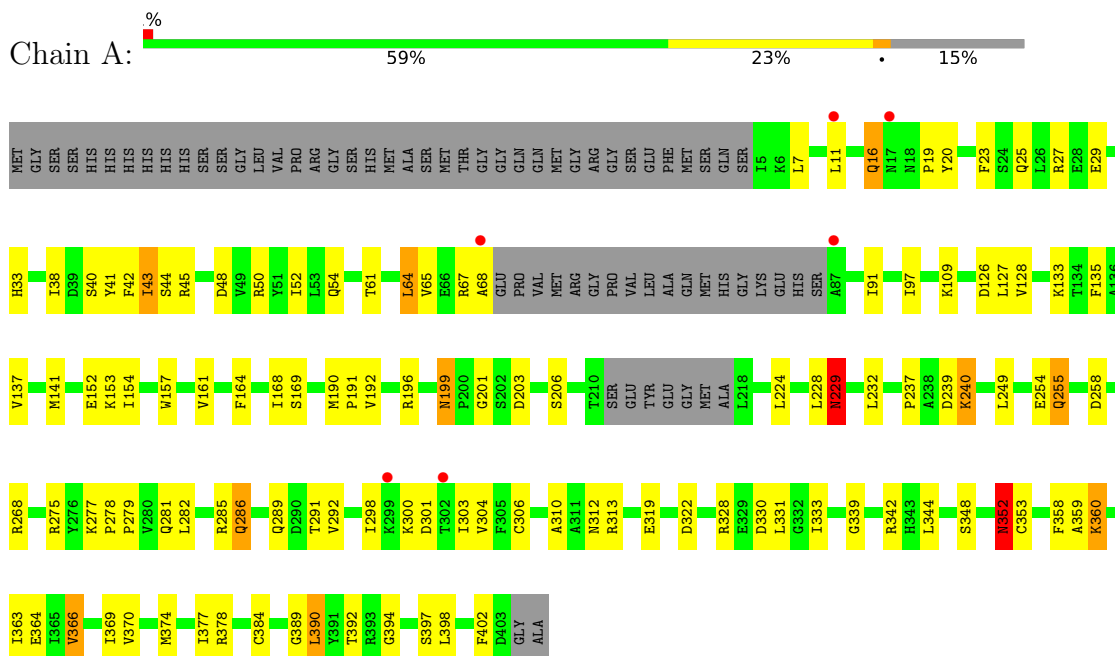
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	O	0	0
			5	5		

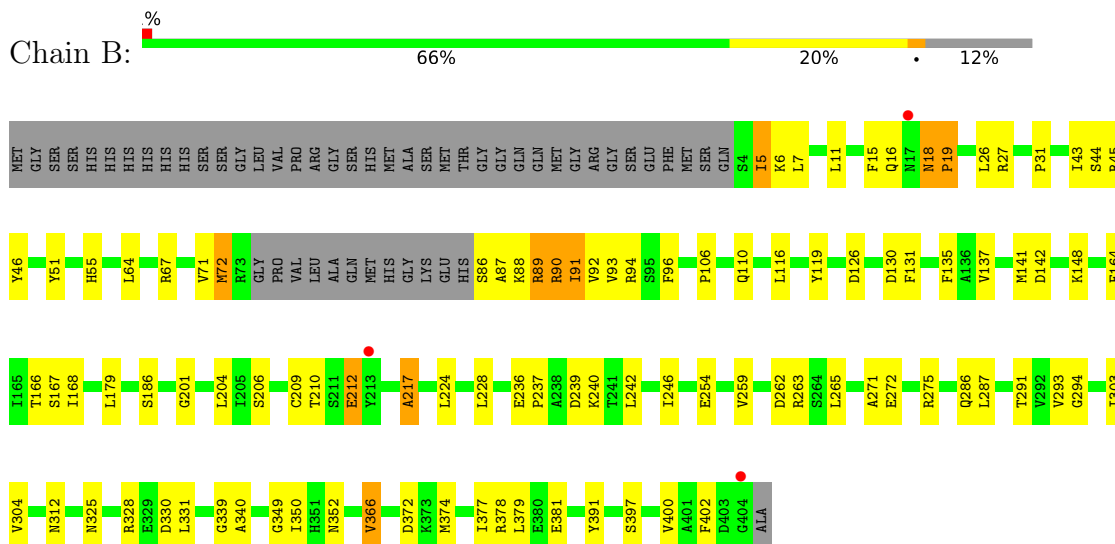
3 Residue-property plots [i](#)

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 cypX



• Molecule 1: Cytochrome P450 cypX



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.95Å 106.90Å 142.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.84 – 3.10 43.84 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.84-3.10) 98.8 (43.84-3.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.62 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.214 , 0.278 0.211 , 0.269	Depositor DCC
R_{free} test set	912 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	66.5	Xtriage
Anisotropy	0.561	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6150	wwPDB-VP
Average B, all atoms (Å ²)	62.0	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 21.32 % 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 7.1894e-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: PIW, HEM, MG

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	0.79	8/3030 (0.3%)	1.06	7/4105 (0.2%)
1	B	0.72	2/3129 (0.1%)	1.12	14/4239 (0.3%)
All	All	0.75	10/6159 (0.2%)	1.09	21/8344 (0.3%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	229	ASN	CG-OD1	6.18	1.35	1.23
1	A	255	GLN	CD-NE2	-5.89	1.20	1.33
1	B	19	PRO	N-CD	5.78	1.55	1.47
1	A	33	HIS	ND1-CE1	5.42	1.38	1.32
1	A	199	ASN	CG-OD1	5.29	1.33	1.23
1	A	16	GLN	CD-OE1	5.27	1.33	1.23
1	A	289	GLN	CD-OE1	5.20	1.33	1.23
1	B	16	GLN	CD-OE1	5.12	1.33	1.23
1	A	352	ASN	CG-OD1	5.10	1.33	1.23
1	A	286	GLN	CD-OE1	5.05	1.33	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	THR	N-CA-C	11.35	125.64	111.69
1	A	7	LEU	N-CA-C	-10.73	100.93	114.56
1	B	209	CYS	N-CA-C	-7.92	102.34	110.97
1	B	89	ARG	N-CA-C	-7.41	104.20	112.57
1	A	366	VAL	CB-CA-C	-7.09	102.89	111.97
1	B	90	ARG	CA-C-N	6.96	134.23	121.70
1	B	90	ARG	C-N-CA	6.96	134.23	121.70
1	A	33	HIS	CB-CG-CD2	-6.52	122.72	131.20
1	A	390	LEU	N-CA-C	-6.17	107.58	114.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	7	LEU	N-CA-C	-6.06	105.85	113.72
1	B	167	SER	N-CA-C	5.71	118.30	110.24
1	B	217	ALA	N-CA-C	5.68	119.23	111.39
1	A	33	HIS	CB-CG-ND1	5.66	131.19	122.70
1	A	43	ILE	N-CA-C	5.65	116.24	107.99
1	B	366	VAL	CB-CA-C	-5.55	104.59	111.70
1	B	210	THR	CB-CA-C	-5.46	100.70	110.70
1	B	18	ASN	CB-CA-C	5.37	120.75	110.17
1	B	72	MET	CB-CA-C	-5.06	109.09	116.53
1	B	349	GLY	N-CA-C	5.05	119.54	110.95
1	A	402	PHE	N-CA-C	5.01	114.86	108.24
1	B	212	GLU	CB-CA-C	5.01	120.40	110.42

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	2968	0	2945	100	0
1	B	3068	0	3027	86	0
2	A	43	0	30	6	0
2	B	43	0	30	1	0
3	A	11	0	8	2	0
3	B	11	0	8	3	0
4	A	1	0	0	0	0
5	A	5	0	0	3	0
All	All	6150	0	6048	187	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 15.

All (187) 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:90:ARG:CB	1:B:91:ILE:HG13	1.50	1.39
1:A:370:VAL:HG13	1:A:374:MET:CE	1.71	1.19
1:A:370:VAL:HG13	1:A:374:MET:HE2	1.15	1.14
1:B:90:ARG:H	1:B:91:ILE:HD12	1.05	1.10
1:A:20:TYR:HA	1:A:23:PHE:CD2	1.87	1.09
1:A:11:LEU:HD11	1:A:168:ILE:HG21	1.22	1.07
1:B:90:ARG:HB3	1:B:91:ILE:CG1	1.83	1.06
1:A:20:TYR:HA	1:A:23:PHE:CE2	1.96	1.00
1:A:11:LEU:CD1	1:A:168:ILE:HG21	1.93	0.98
1:B:339:GLY:HA2	1:B:352:ASN:ND2	1.77	0.98
1:A:65:VAL:HG23	1:A:229:ASN:OD1	1.64	0.98
1:A:135:PHE:CZ	1:A:366:VAL:CG2	2.48	0.96
1:B:90:ARG:H	1:B:91:ILE:CD1	1.78	0.96
1:B:88:LYS:C	1:B:91:ILE:HD12	1.91	0.95
1:B:90:ARG:CA	1:B:91:ILE:HG13	1.98	0.94
1:B:90:ARG:CB	1:B:91:ILE:CG1	2.43	0.93
1:B:90:ARG:HB3	1:B:91:ILE:HG13	0.94	0.93
1:A:342:ARG:HB2	5:A:410:HOH:O	1.70	0.90
1:B:135:PHE:CZ	1:B:366:VAL:CG2	2.55	0.90
1:A:370:VAL:CG1	1:A:374:MET:CE	2.49	0.90
1:A:135:PHE:CE2	1:A:366:VAL:HG21	2.08	0.88
1:B:90:ARG:N	1:B:91:ILE:HD12	1.89	0.86
1:A:20:TYR:HA	1:A:23:PHE:HD2	1.42	0.81
1:B:5:ILE:CB	1:B:6:LYS:HA	2.11	0.80
1:A:27:ARG:HB3	1:A:44:SER:OG	1.82	0.80
1:B:90:ARG:O	1:B:93:VAL:HB	1.81	0.80
1:B:135:PHE:CE2	1:B:366:VAL:HG21	2.17	0.79
1:A:43:ILE:HD13	1:A:52:ILE:HD11	1.66	0.78
1:A:135:PHE:CZ	1:A:366:VAL:HG22	2.17	0.78
1:A:237:PRO:HB2	2:A:406:HEM:HBB2	1.65	0.78
1:B:339:GLY:HA2	1:B:352:ASN:HD22	1.49	0.76
1:A:268:ARG:HG2	1:A:333:ILE:HG21	1.70	0.74
1:B:242:LEU:HD21	1:B:366:VAL:HG11	1.70	0.73
1:A:199:ASN:O	1:A:199:ASN:OD1	2.06	0.73
1:B:88:LYS:C	1:B:91:ILE:CD1	2.62	0.73
1:A:19:PRO:C	1:A:23:PHE:CE2	2.68	0.72
1:B:242:LEU:CD2	1:B:366:VAL:HG11	2.19	0.72
1:A:127:LEU:HD21	1:A:374:MET:HE1	1.72	0.71
1:A:374:MET:HE3	1:A:377:ILE:HD11	1.72	0.70
1:A:20:TYR:CA	1:A:23:PHE:CE2	2.73	0.70
2:A:406:HEM:HHD	2:A:406:HEM:HBC2	1.72	0.70
1:A:97:ILE:CG2	1:A:358:PHE:HB2	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:GLN:HA	1:A:303:ILE:HG12	1.75	0.68
1:B:90:ARG:N	1:B:91:ILE:HB	2.09	0.68
1:A:201:GLY:H	1:A:206:SER:HB3	1.59	0.68
1:B:90:ARG:N	1:B:91:ILE:CG1	2.58	0.67
1:B:90:ARG:CA	1:B:91:ILE:CG1	2.71	0.66
1:B:64:LEU:HD21	3:B:407:PIW:H5	1.76	0.66
1:A:201:GLY:H	1:A:206:SER:CB	2.07	0.66
1:B:96:PHE:CE2	1:B:204:LEU:HB2	2.30	0.66
1:A:192:VAL:O	1:A:196:ARG:HG3	1.96	0.65
1:B:11:LEU:HD22	1:B:168:ILE:HD11	1.78	0.65
1:A:43:ILE:HD13	1:A:52:ILE:CD1	2.26	0.65
1:B:135:PHE:CZ	1:B:366:VAL:HG22	2.31	0.65
1:A:353:CYS:HB2	2:A:406:HEM:NA	2.11	0.65
1:A:38:ILE:HD12	1:A:40:SER:HB2	1.81	0.63
1:B:27:ARG:HB3	1:B:44:SER:OG	1.99	0.63
1:A:286:GLN:HB2	1:A:303:ILE:HG12	1.80	0.62
1:A:38:ILE:HD11	1:A:42:PHE:HE2	1.65	0.62
1:A:278:PRO:O	1:A:281:GLN:NE2	2.33	0.61
1:A:370:VAL:CG1	1:A:374:MET:HE3	2.29	0.60
1:A:229:ASN:ND2	2:A:406:HEM:O2D	2.33	0.60
1:A:286:GLN:CA	1:A:303:ILE:HG12	2.30	0.60
1:A:20:TYR:CA	1:A:23:PHE:HE2	2.14	0.60
1:B:328:ARG:HG3	1:B:331:LEU:HB2	1.83	0.60
1:A:19:PRO:O	1:A:23:PHE:CE2	2.55	0.59
1:A:20:TYR:HA	1:A:23:PHE:HE2	1.62	0.59
1:B:88:LYS:HB3	1:B:91:ILE:CD1	2.32	0.59
1:B:88:LYS:HB3	1:B:91:ILE:HD11	1.84	0.59
1:A:255:GLN:OE1	1:B:340:ALA:HB1	2.02	0.59
1:B:90:ARG:NH2	1:B:352:ASN:O	2.30	0.59
1:B:263:ARG:NH2	1:B:372:ASP:OD1	2.36	0.58
1:A:286:GLN:CB	1:A:303:ILE:HG12	2.34	0.58
1:B:71:VAL:CG1	1:B:179:LEU:HA	2.34	0.58
1:A:50:ARG:O	1:A:54:GLN:HG2	2.03	0.57
1:B:88:LYS:O	1:B:91:ILE:CD1	2.52	0.57
1:A:168:ILE:HG13	1:A:169:SER:N	2.18	0.57
1:A:313:ARG:HD2	1:A:322:ASP:OD1	2.04	0.57
1:B:90:ARG:H	1:B:91:ILE:CG1	2.16	0.57
1:B:212:GLU:HB3	1:B:217:ALA:H	1.69	0.57
1:B:43:ILE:HD12	1:B:304:VAL:HB	1.87	0.57
1:A:133:LYS:O	1:A:137:VAL:HG23	2.05	0.56
1:A:127:LEU:HD12	1:A:398:LEU:HD23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ILE:H	1:B:94:ARG:H	1.53	0.56
1:A:23:PHE:HD1	1:A:310:ALA:HB2	1.71	0.56
1:A:27:ARG:CB	1:A:44:SER:OG	2.54	0.56
1:B:142:ASP:OD1	1:B:148:LYS:HE2	2.06	0.55
1:B:137:VAL:O	1:B:141:MET:HG3	2.07	0.55
1:A:161:VAL:O	1:A:164:PHE:HB3	2.06	0.55
1:B:272:GLU:HG2	1:B:325:ASN:O	2.05	0.55
1:B:286:GLN:HG3	1:B:303:ILE:HG22	1.89	0.54
1:B:239:ASP:OD1	1:B:240:LYS:N	2.38	0.54
1:B:378:ARG:HG2	1:B:379:LEU:N	2.23	0.54
1:B:90:ARG:N	1:B:91:ILE:CB	2.70	0.53
1:A:203:ASP:OD1	1:A:206:SER:HB2	2.08	0.53
1:A:255:GLN:O	1:A:258:ASP:HB2	2.07	0.53
1:B:15:PHE:O	1:B:18:ASN:O	2.25	0.53
1:B:328:ARG:HD3	1:B:330:ASP:OD1	2.08	0.53
1:A:203:ASP:OD1	1:A:206:SER:CB	2.57	0.53
1:B:86:SER:OG	1:B:87:ALA:N	2.39	0.53
1:A:45:ARG:HB2	1:A:48:ASP:OD2	2.08	0.52
1:A:190:MET:N	1:A:191:PRO:HD2	2.25	0.52
1:A:190:MET:HE2	1:A:224:LEU:HD22	1.90	0.52
1:B:237:PRO:HB2	2:B:406:HEM:HBB2	1.92	0.52
1:A:240:LYS:HG2	1:A:394:GLY:HA3	1.91	0.52
1:A:254:GLU:HB2	5:A:413:HOH:O	2.11	0.51
1:A:154:ILE:HD13	1:A:157:TRP:CE3	2.46	0.51
1:B:287:LEU:HD23	1:B:291:THR:HG22	1.93	0.51
1:A:330:ASP:HB2	1:A:342:ARG:HH21	1.75	0.50
1:A:27:ARG:CA	1:A:44:SER:OG	2.60	0.50
1:A:64:LEU:N	1:A:229:ASN:HD21	2.10	0.50
1:B:43:ILE:CD1	1:B:304:VAL:HB	2.41	0.50
1:B:126:ASP:OD2	1:B:397:SER:HB2	2.12	0.49
1:A:19:PRO:O	1:A:23:PHE:CD2	2.66	0.49
1:B:242:LEU:HD21	1:B:366:VAL:CG1	2.40	0.49
1:A:168:ILE:HG13	1:A:169:SER:H	1.76	0.49
1:B:72:MET:HE1	1:B:228:LEU:HD13	1.94	0.49
1:A:16:GLN:HG3	1:A:390:LEU:HD12	1.95	0.48
1:B:5:ILE:CB	1:B:6:LYS:CA	2.85	0.48
1:B:88:LYS:O	1:B:91:ILE:HD12	2.11	0.48
1:A:328:ARG:HG3	1:A:331:LEU:HB2	1.94	0.48
1:A:41:TYR:HB2	1:A:304:VAL:HG12	1.96	0.48
1:A:20:TYR:N	1:A:23:PHE:CE2	2.82	0.48
1:B:201:GLY:H	1:B:206:SER:CB	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:LEU:HD21	3:B:407:PIW:C5	2.43	0.48
1:A:128:VAL:HB	1:A:397:SER:HA	1.95	0.47
1:A:282:LEU:HA	1:A:306:CYS:O	2.15	0.47
1:A:359:ALA:O	1:A:360:LYS:C	2.58	0.47
1:B:166:THR:HG22	1:B:391:TYR:HB3	1.95	0.47
1:B:88:LYS:O	1:B:91:ILE:HD13	2.15	0.47
1:A:135:PHE:CE2	1:A:366:VAL:CG2	2.78	0.47
2:A:406:HEM:C1A	3:A:407:PIW:H4	2.50	0.47
1:A:389:GLY:HA3	1:A:392:THR:O	2.14	0.47
1:B:186:SER:HB2	1:B:224:LEU:HD21	1.97	0.46
1:A:25:GLN:NE2	1:A:29:GLU:OE1	2.49	0.46
1:B:275:ARG:HA	1:B:312:ASN:ND2	2.31	0.46
1:A:61:THR:HB	1:A:285:ARG:HD3	1.97	0.46
1:A:339:GLY:HA2	1:A:352:ASN:OD1	2.15	0.46
1:B:339:GLY:HA2	1:B:352:ASN:HD21	1.73	0.45
1:A:328:ARG:HD2	1:A:331:LEU:HD13	1.98	0.45
1:B:259:VAL:O	1:B:262:ASP:O	2.34	0.45
1:B:378:ARG:NH2	1:B:381:GLU:HG2	2.31	0.45
1:A:64:LEU:H	1:A:64:LEU:HG	1.48	0.45
1:A:291:THR:HG22	1:A:292:VAL:N	2.32	0.45
1:B:271:ALA:HB3	1:B:331:LEU:HD21	1.98	0.45
1:A:20:TYR:N	1:A:23:PHE:HE2	2.14	0.45
1:B:51:TYR:CE1	1:B:55:HIS:CE1	3.05	0.45
1:A:20:TYR:CZ	1:A:277:LYS:HD3	2.52	0.45
1:B:67:ARG:O	1:B:164:PHE:HE2	2.00	0.45
1:B:331:LEU:O	1:B:331:LEU:HG	2.15	0.45
1:B:378:ARG:HH22	1:B:381:GLU:HG2	1.81	0.45
1:A:126:ASP:C	1:A:126:ASP:OD1	2.59	0.44
1:A:109:LYS:HG3	1:A:369:ILE:HD11	1.99	0.44
1:B:339:GLY:CA	1:B:352:ASN:ND2	2.65	0.44
1:A:54:GLN:NE2	1:A:348:SER:OG	2.52	0.43
1:B:236:GLU:HG3	3:B:407:PIW:C8	2.48	0.43
1:B:116:LEU:HG	1:B:131:PHE:CE1	2.54	0.43
1:B:119:TYR:CZ	1:B:130:ASP:HB3	2.54	0.43
1:A:300:LYS:O	1:A:301:ASP:HB2	2.19	0.43
1:B:239:ASP:CG	1:B:240:LYS:N	2.77	0.43
1:B:89:ARG:C	1:B:91:ILE:HB	2.43	0.43
1:B:374:MET:HE1	1:B:400:VAL:HG21	2.01	0.42
1:B:86:SER:C	1:B:88:LYS:H	2.28	0.42
1:A:358:PHE:HD2	2:A:406:HEM:HMC3	1.84	0.42
1:B:46:TYR:CD1	1:B:46:TYR:C	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:LEU:CD2	3:A:407:PIW:H5	2.49	0.42
1:A:27:ARG:N	1:A:44:SER:OG	2.52	0.42
1:A:67:ARG:O	1:A:68:ALA:HB3	2.19	0.42
1:B:263:ARG:C	1:B:265:LEU:N	2.78	0.42
1:A:20:TYR:CD1	1:A:23:PHE:CE2	3.09	0.41
1:A:249:LEU:HD23	1:A:249:LEU:HA	1.94	0.41
1:A:342:ARG:CB	5:A:410:HOH:O	2.46	0.41
1:B:242:LEU:HD22	1:B:366:VAL:HG11	1.99	0.41
1:A:374:MET:O	1:A:377:ILE:HG13	2.19	0.41
1:B:31:PRO:HG3	1:B:45:ARG:HE	1.85	0.41
1:B:135:PHE:CE2	1:B:366:VAL:CG2	2.84	0.41
1:A:239:ASP:OD1	1:A:240:LYS:N	2.53	0.41
1:A:278:PRO:HA	1:A:279:PRO:HD3	1.86	0.41
1:B:374:MET:HB3	1:B:402:PHE:CG	2.56	0.41
1:A:61:THR:HB	1:A:285:ARG:CD	2.51	0.41
1:A:137:VAL:O	1:A:141:MET:HG3	2.21	0.40
1:A:228:LEU:O	1:A:232:LEU:HG	2.21	0.40
1:A:152:GLU:O	1:A:153:LYS:C	2.64	0.40
1:B:106:PRO:O	1:B:110:GLN:HG3	2.21	0.40
1:B:90:ARG:N	1:B:91:ILE:CD1	2.57	0.40
1:A:275:ARG:HA	1:A:312:ASN:HD22	1.87	0.40
1:A:363:ILE:O	1:A:364:GLU:C	2.65	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	369/441 (84%)	330 (89%)	39 (11%)	0	100	100
1	B	385/441 (87%)	353 (92%)	28 (7%)	4 (1%)	12	41
All	All	754/882 (86%)	683 (91%)	67 (9%)	4 (0%)	24	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	5	ILE
1	B	91	ILE
1	B	19	PRO
1	B	294	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	327/380 (86%)	316 (97%)	11 (3%)	32	63
1	B	336/380 (88%)	329 (98%)	7 (2%)	47	71
All	All	663/760 (87%)	645 (97%)	18 (3%)	39	67

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	LEU
1	A	91	ILE
1	A	229	ASN
1	A	240	LYS
1	A	298	ILE
1	A	319	GLU
1	A	344	LEU
1	A	352	ASN
1	A	360	LYS
1	A	378	ARG
1	A	384	CYS
1	B	26	LEU
1	B	92	VAL
1	B	246	ILE
1	B	254	GLU
1	B	293	VAL
1	B	350	ILE
1	B	377	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	199	ASN
1	A	312	ASN
1	A	327	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	B	406	1	50,50,50	1.84	9 (18%)	67,82,82	1.42	9 (13%)
2	HEM	A	406	1	50,50,50	2.02	15 (30%)	67,82,82	1.55	9 (13%)
3	PIW	B	407	-	12,12,12	1.67	2 (16%)	15,15,15	2.58	8 (53%)
3	PIW	A	407	-	12,12,12	1.80	2 (16%)	15,15,15	2.42	8 (53%)

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	B	406	1	-	7/14/54/54	-
2	HEM	A	406	1	-	10/14/54/54	-
3	PIW	B	407	-	-	2/4/4/4	0/2/2/2
3	PIW	A	407	-	-	2/4/4/4	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	406	HEM	C3D-C2D	7.93	1.53	1.36
2	B	406	HEM	C3D-C2D	7.49	1.52	1.36
3	A	407	PIW	C6-N1	-4.58	1.35	1.43
3	B	407	PIW	C6-N1	-4.31	1.36	1.43
2	A	406	HEM	FE-NB	3.93	2.07	1.94
2	A	406	HEM	FE-NC	3.31	2.06	1.95
2	A	406	HEM	FE-ND	3.26	2.04	1.94
2	A	406	HEM	CAC-C3C	3.23	1.56	1.47
2	A	406	HEM	FE-NA	3.20	2.05	1.95
2	A	406	HEM	CAB-C3B	3.20	1.55	1.47
2	B	406	HEM	C3C-C2C	-3.18	1.30	1.37
2	B	406	HEM	FE-NC	3.04	2.05	1.95
2	B	406	HEM	CAB-C3B	2.95	1.55	1.47
2	B	406	HEM	C2A-C3A	-2.94	1.31	1.38
2	A	406	HEM	CMD-C2D	2.65	1.56	1.50
2	B	406	HEM	FE-NA	2.56	2.03	1.95
2	A	406	HEM	O1D-CGD	2.44	1.30	1.22
2	A	406	HEM	C2A-C3A	-2.42	1.32	1.38
2	A	406	HEM	CMA-C3A	2.27	1.55	1.50
2	A	406	HEM	CMC-C2C	2.18	1.55	1.50
3	A	407	PIW	C5-N1	-2.16	1.34	1.38
2	A	406	HEM	CAD-C3D	2.14	1.56	1.51
2	B	406	HEM	CAD-C3D	2.13	1.56	1.51
2	A	406	HEM	CMB-C2B	2.12	1.55	1.50
2	B	406	HEM	CMC-C2C	2.09	1.55	1.50
3	B	407	PIW	C5-N1	-2.00	1.34	1.38
2	A	406	HEM	O1A-CGA	2.00	1.28	1.22
2	B	406	HEM	FE-ND	2.00	2.01	1.94

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	407	PIW	C5-N1-C2	5.48	114.52	106.40
2	A	406	HEM	C4D-ND-C1D	5.41	111.61	105.21
3	A	407	PIW	C5-N1-C2	5.38	114.38	106.40
2	B	406	HEM	C4D-ND-C1D	4.75	110.84	105.21
3	A	407	PIW	C6-N1-C5	-3.73	121.37	126.84
2	A	406	HEM	CBA-CAA-C2A	-3.54	102.75	112.53
2	A	406	HEM	CAD-C3D-C4D	3.49	130.77	124.70
3	B	407	PIW	C11-C6-N1	3.45	124.58	119.80
3	B	407	PIW	C6-N1-C5	-3.42	121.84	126.84
2	A	406	HEM	CMD-C2D-C1D	3.34	130.26	125.03
3	B	407	PIW	C8-C7-C6	3.34	123.65	119.68
2	B	406	HEM	CAD-C3D-C4D	3.31	130.46	124.70
2	B	406	HEM	CAA-CBA-CGA	-3.29	104.93	113.67
2	B	406	HEM	CMD-C2D-C1D	3.21	130.05	125.03
3	A	407	PIW	C8-C7-C6	3.13	123.41	119.68
2	B	406	HEM	O2D-CGD-CBD	3.06	123.66	114.00
2	A	406	HEM	CAD-CBD-CGD	-3.01	105.68	113.67
2	B	406	HEM	O1D-CGD-CBD	-2.89	113.94	123.09
3	A	407	PIW	C11-C6-N1	2.81	123.69	119.80
3	B	407	PIW	C11-C6-C7	-2.70	114.03	119.18
3	B	407	PIW	C10-C11-C6	2.69	122.88	119.68
3	B	407	PIW	N1-C2-N3	-2.54	104.62	111.13
2	B	406	HEM	C4C-C3C-C2C	2.43	108.92	106.81
3	A	407	PIW	C10-C11-C6	2.36	122.49	119.68
3	A	407	PIW	N1-C2-N3	-2.32	105.18	111.13
3	A	407	PIW	C11-C6-C7	-2.26	114.87	119.18
3	B	407	PIW	C6-N1-C2	-2.26	123.51	127.20
2	A	406	HEM	C1B-NB-C4B	2.18	107.79	105.21
3	A	407	PIW	C4-C5-N1	-2.13	102.85	106.70
2	A	406	HEM	C3B-C2B-C1B	2.10	107.99	106.41
2	B	406	HEM	CHB-C1B-NB	2.06	126.91	124.37
2	A	406	HEM	CAC-C3C-C4C	2.06	129.73	124.82
2	A	406	HEM	CHC-C1C-NC	2.02	126.65	124.45
2	B	406	HEM	O1A-CGA-CBA	-2.01	116.73	123.09

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	406	HEM	C2B-C3B-CAB-CBB
2	A	406	HEM	C4B-C3B-CAB-CBB
2	A	406	HEM	C3D-CAD-CBD-CGD
2	A	406	HEM	C4C-C3C-CAC-CBC

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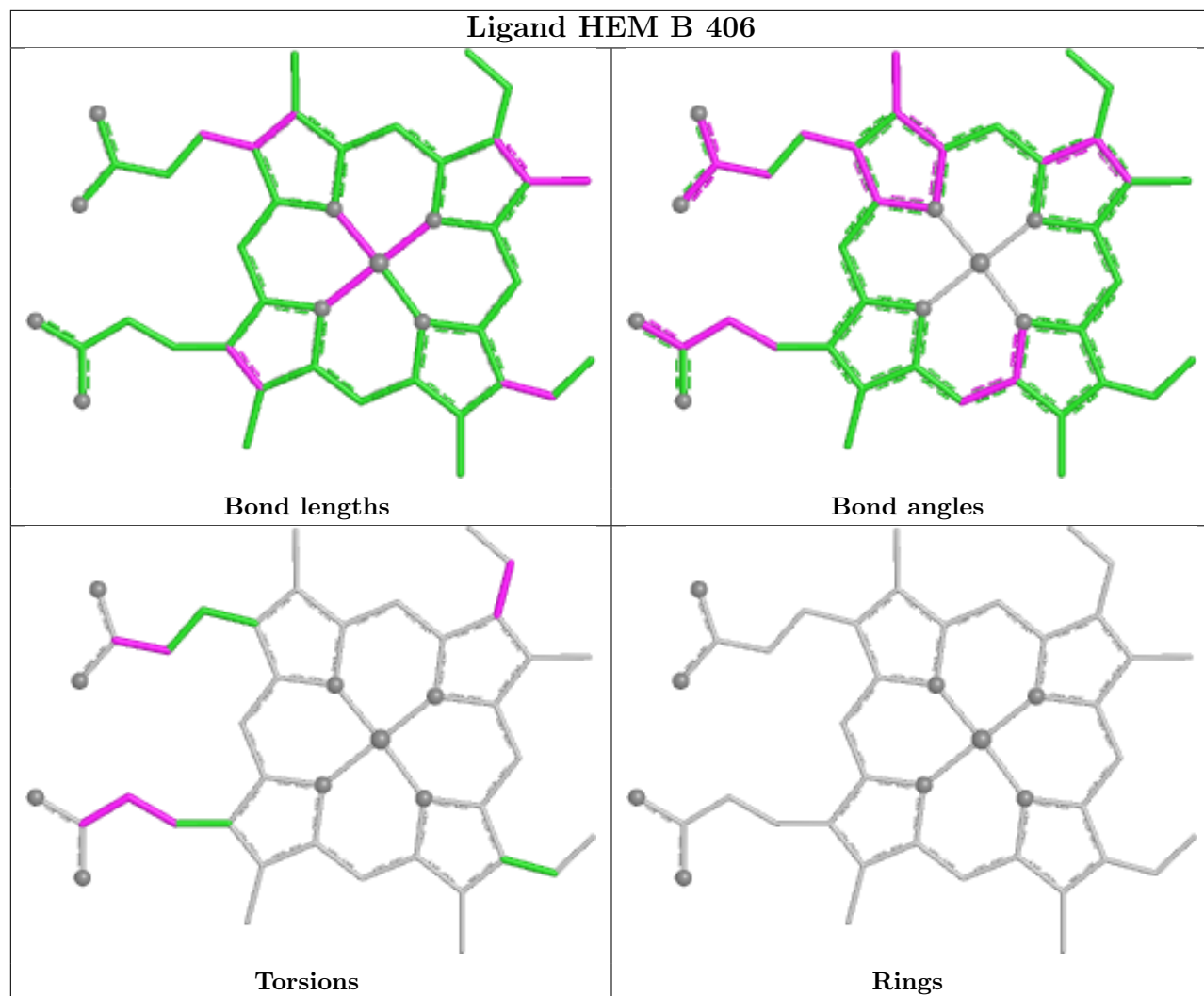
Mol	Chain	Res	Type	Atoms
2	A	406	HEM	C2D-C3D-CAD-CBD
2	A	406	HEM	C4D-C3D-CAD-CBD
3	B	407	PIW	C7-C6-N1-C5
2	B	406	HEM	C2A-CAA-CBA-CGA
2	B	406	HEM	CAD-CBD-CGD-O1D
2	B	406	HEM	CAD-CBD-CGD-O2D
2	A	406	HEM	CAA-CBA-CGA-O1A
3	A	407	PIW	C7-C6-N1-C5
2	A	406	HEM	CAA-CBA-CGA-O2A
3	B	407	PIW	C11-C6-N1-C5
2	B	406	HEM	CAA-CBA-CGA-O1A
2	B	406	HEM	CAA-CBA-CGA-O2A
2	B	406	HEM	C2C-C3C-CAC-CBC
2	B	406	HEM	C4C-C3C-CAC-CBC
2	A	406	HEM	CAD-CBD-CGD-O1D
2	A	406	HEM	CAD-CBD-CGD-O2D
3	A	407	PIW	C11-C6-N1-C5

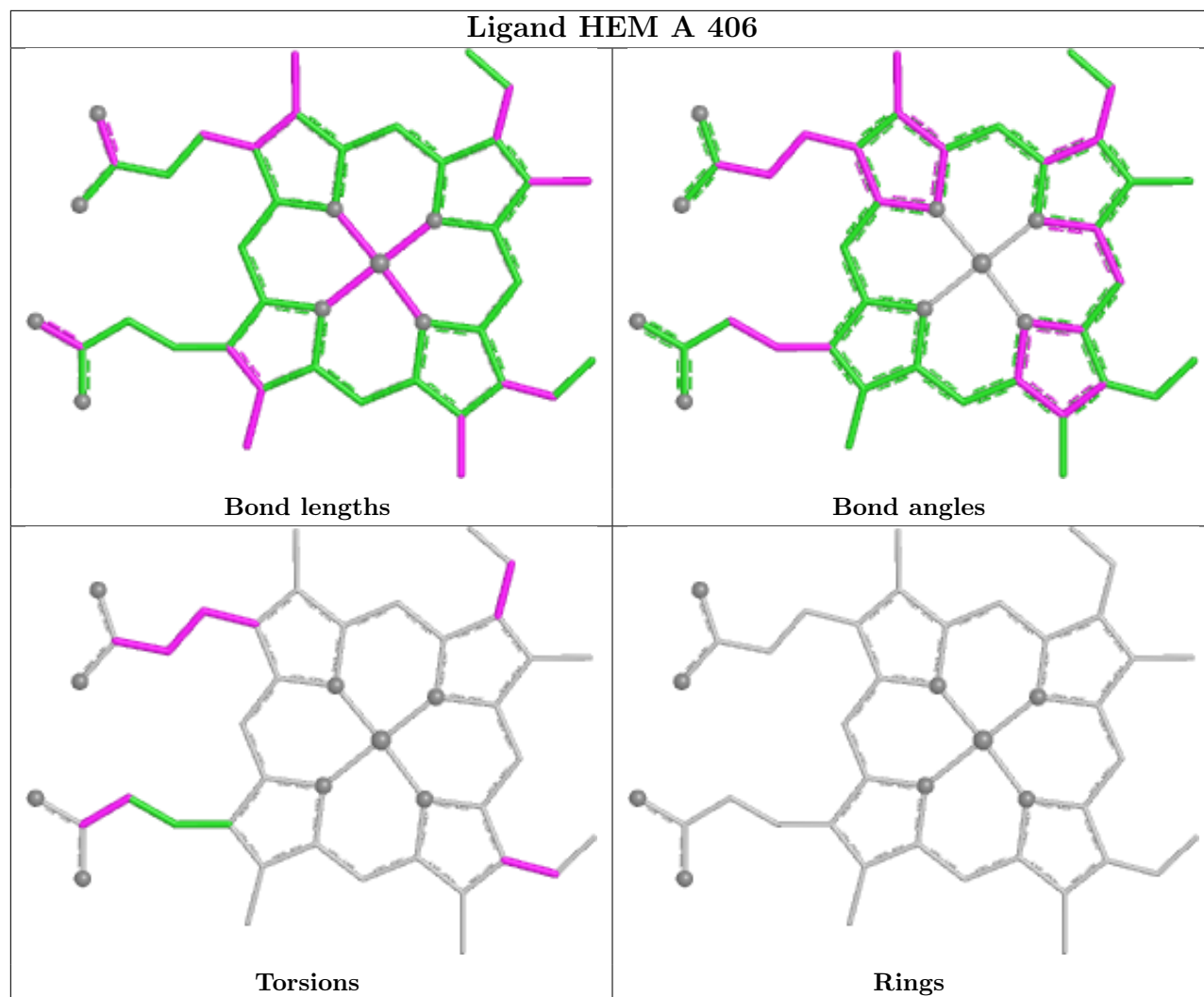
There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	406	HEM	1	0
2	A	406	HEM	6	0
3	B	407	PIW	3	0
3	A	407	PIW	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	374/441 (84%)	-0.21	6 (1%)	70 49	34, 59, 109, 162	2 (0%)
1	B	389/441 (88%)	-0.26	3 (0%)	82 65	34, 57, 92, 114	1 (0%)
All	All	763/882 (86%)	-0.23	9 (1%)	76 58	34, 58, 99, 162	3 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	ALA	3.9
1	A	17	ASN	3.1
1	A	302	THR	2.8
1	B	213	TYR	2.7
1	A	299	LYS	2.6
1	A	11	LEU	2.6
1	B	404	GLY	2.1
1	B	17	ASN	2.1
1	A	87	ALA	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,

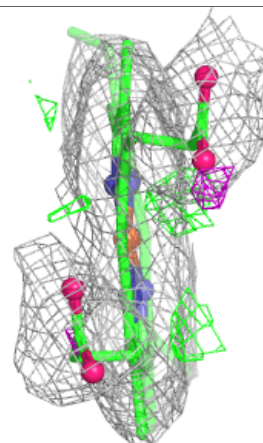
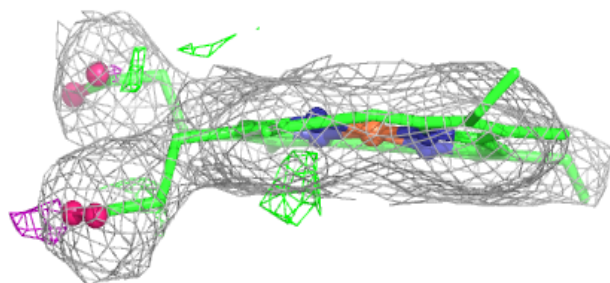
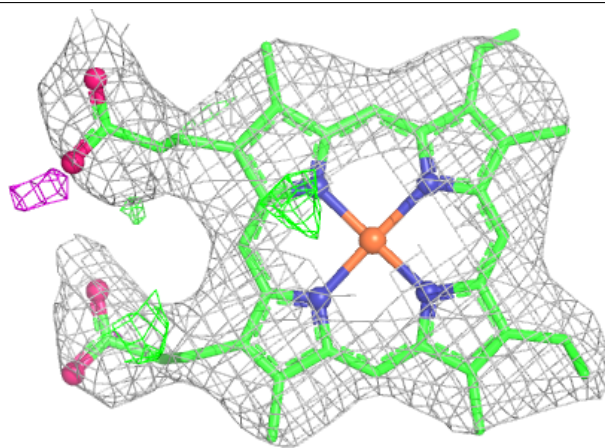
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

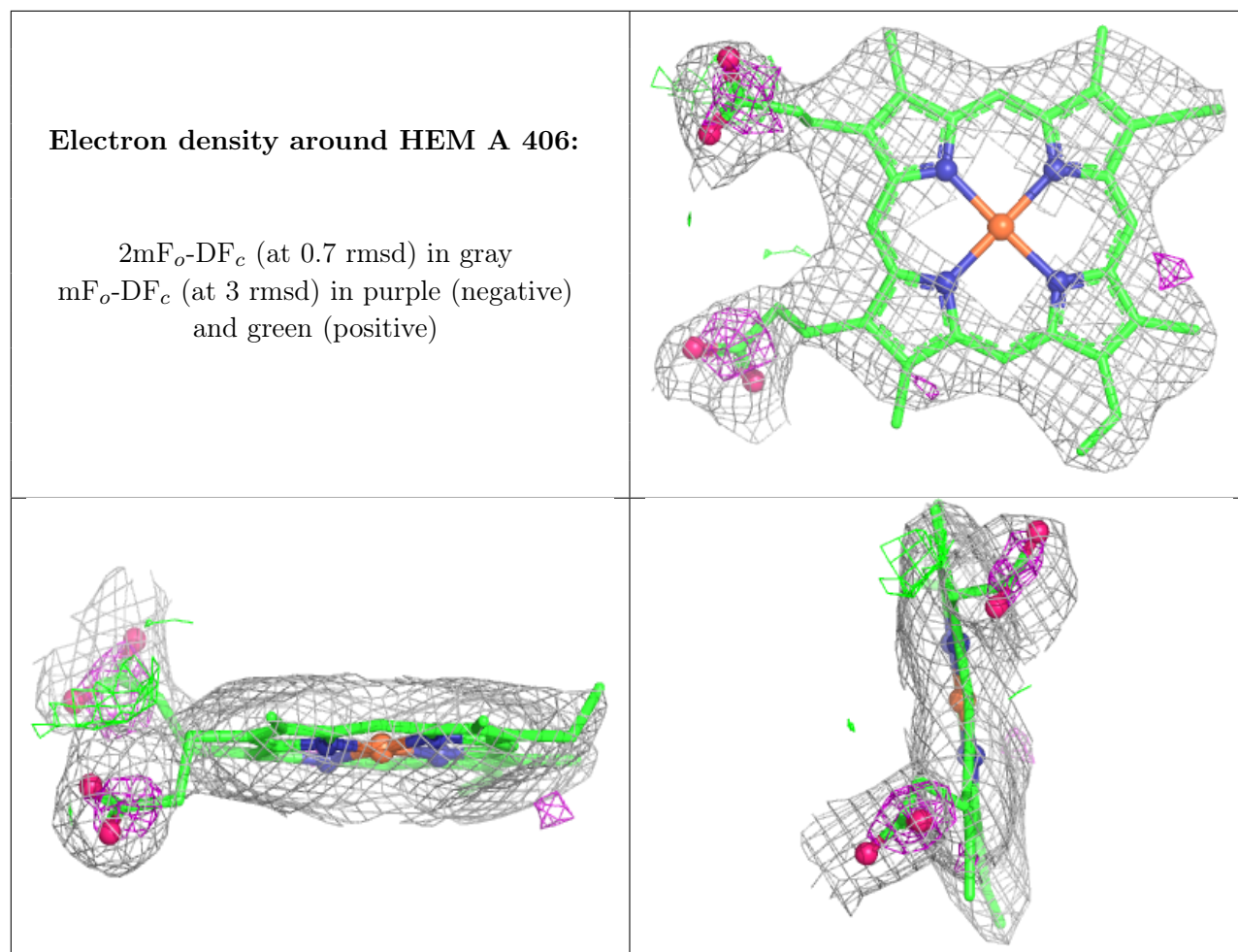
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	A	408	1/1	0.59	0.44	72,72,72,72	0
3	PIW	A	407	11/11	0.92	0.14	61,62,63,64	0
3	PIW	B	407	11/11	0.95	0.12	41,44,47,47	0
2	HEM	B	406	43/43	0.97	0.08	16,19,37,38	0
2	HEM	A	406	43/43	0.97	0.08	17,20,40,42	0

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

Electron density around HEM B 406:

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.