



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:38 PM UTC

PDB ID : 4PK5 / pdb_00004pk5
Title : Crystal structure of the indoleamine 2,3-dioxygenase 1 (IDO1) complexed with Amg-1
Authors : Kohno, T.; Tojo, S.; Ishii, T.
Deposited on : 2014-05-13
Resolution : 2.79 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

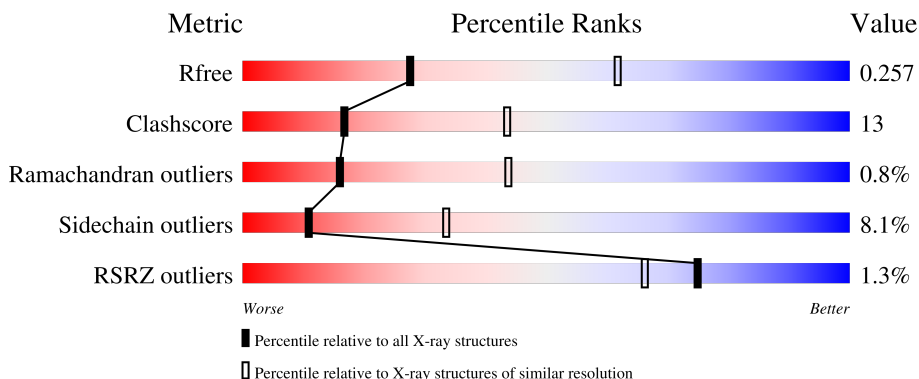
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	423	
1	B	423	

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	PKJ	B	502	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6064 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 Indoleamine 2,3-dioxygenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2956	1899	504	536	17			
1	B	373	Total	C	N	O	S	0	0	0
			2956	1899	504	536	17			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P14902
A	-18	GLY	-	expression tag	UNP P14902
A	-17	SER	-	expression tag	UNP P14902
A	-16	SER	-	expression tag	UNP P14902
A	-15	HIS	-	expression tag	UNP P14902
A	-14	HIS	-	expression tag	UNP P14902
A	-13	HIS	-	expression tag	UNP P14902
A	-12	HIS	-	expression tag	UNP P14902
A	-11	HIS	-	expression tag	UNP P14902
A	-10	HIS	-	expression tag	UNP P14902
A	-9	SER	-	expression tag	UNP P14902
A	-8	SER	-	expression tag	UNP P14902
A	-7	GLY	-	expression tag	UNP P14902
A	-6	LEU	-	expression tag	UNP P14902
A	-5	VAL	-	expression tag	UNP P14902
A	-4	PRO	-	expression tag	UNP P14902
A	-3	ARG	-	expression tag	UNP P14902
A	-2	GLY	-	expression tag	UNP P14902
A	-1	SER	-	expression tag	UNP P14902
A	0	HIS	-	expression tag	UNP P14902
B	-19	MET	-	expression tag	UNP P14902
B	-18	GLY	-	expression tag	UNP P14902
B	-17	SER	-	expression tag	UNP P14902
B	-16	SER	-	expression tag	UNP P14902
B	-15	HIS	-	expression tag	UNP P14902

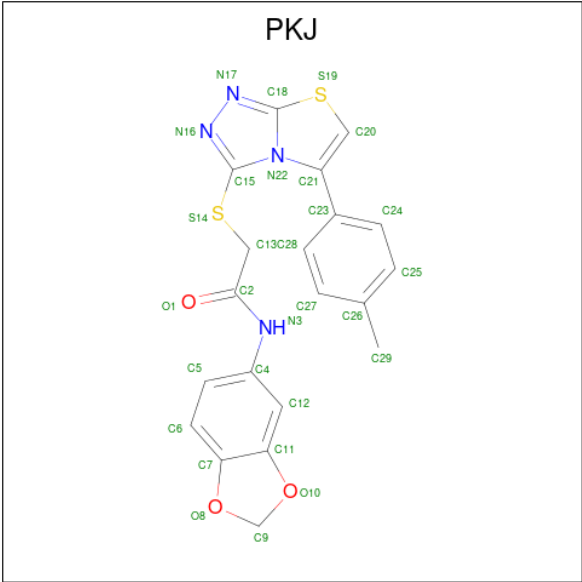
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP P14902
B	-13	HIS	-	expression tag	UNP P14902
B	-12	HIS	-	expression tag	UNP P14902
B	-11	HIS	-	expression tag	UNP P14902
B	-10	HIS	-	expression tag	UNP P14902
B	-9	SER	-	expression tag	UNP P14902
B	-8	SER	-	expression tag	UNP P14902
B	-7	GLY	-	expression tag	UNP P14902
B	-6	LEU	-	expression tag	UNP P14902
B	-5	VAL	-	expression tag	UNP P14902
B	-4	PRO	-	expression tag	UNP P14902
B	-3	ARG	-	expression tag	UNP P14902
B	-2	GLY	-	expression tag	UNP P14902
B	-1	SER	-	expression tag	UNP P14902
B	0	HIS	-	expression tag	UNP P14902

- # HEM

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

- 



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			29	20	4	3	2		
3	B	1	Total	C	N	O	S	0	0
			29	20	4	3	2		

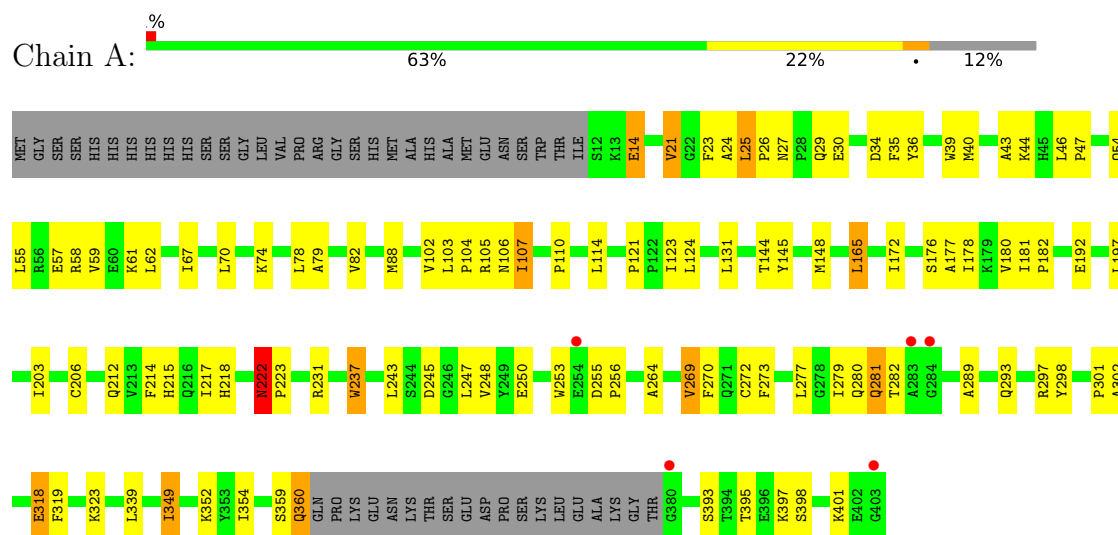
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	B	3	Total	O	0	0
			3	3		

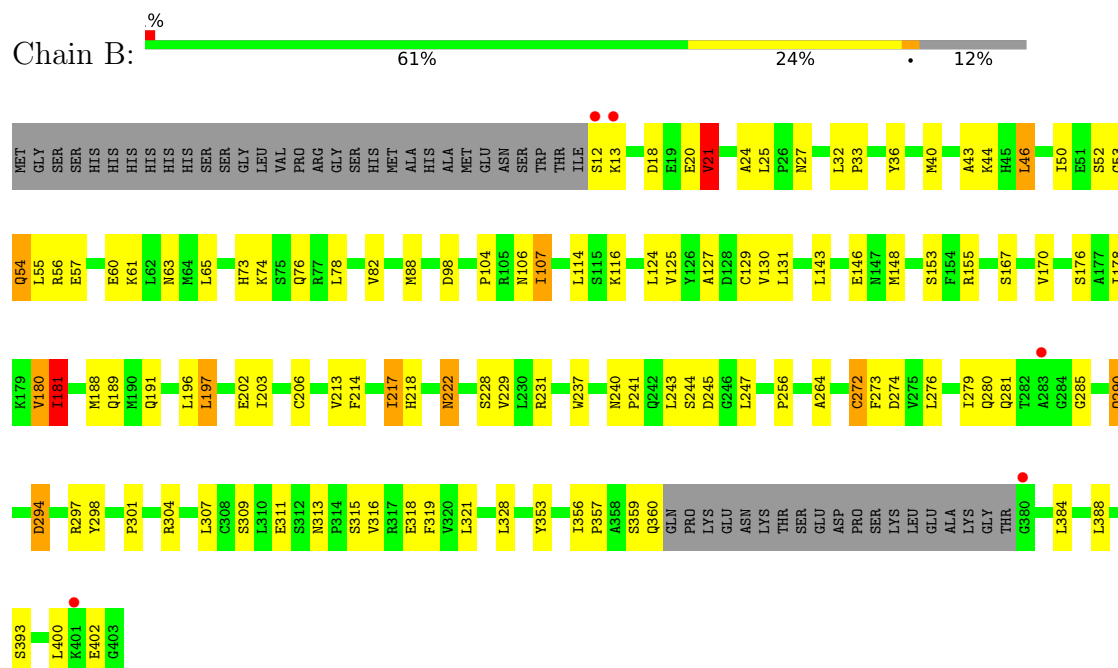
3 Residue-property plots [i](#)

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: Indoleamine 2,3-dioxygenase 1



• Molecule 1: Indoleamine 2,3-dioxygenase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.80Å 90.41Å 131.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.55 – 2.79 74.55 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.0 (74.55-2.79) 99.0 (74.55-2.79)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.185 , 0.256 0.185 , 0.257	Depositor DCC
R_{free} test set	1255 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	61.6	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6064	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.86	0/3024	1.08	7/4087 (0.2%)
1	B	0.74	0/3024	1.15	11/4087 (0.3%)
All	All	0.80	0/6048	1.11	18/8174 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	313	ASN	CA-C-N	-13.93	105.48	120.66
1	B	313	ASN	C-N-CA	-13.93	105.48	120.66
1	B	21	VAL	CB-CA-C	7.41	120.69	111.65
1	A	222	ASN	CA-C-N	6.38	127.82	119.84
1	A	222	ASN	C-N-CA	6.38	127.82	119.84
1	B	222	ASN	CA-C-N	6.24	127.64	119.84
1	B	222	ASN	C-N-CA	6.24	127.64	119.84
1	A	54	GLN	N-CA-C	6.24	120.22	111.30
1	B	402	GLU	N-CA-C	-5.93	106.01	113.72
1	A	172	ILE	CB-CA-C	-5.74	104.39	112.14
1	B	130	VAL	CB-CA-C	-5.65	106.07	111.44
1	A	172	ILE	N-CA-C	5.63	116.36	110.62
1	B	25	LEU	CA-C-N	5.48	124.94	119.24
1	B	25	LEU	C-N-CA	5.48	124.94	119.24
1	A	25	LEU	CA-C-N	5.41	124.86	119.24
1	A	25	LEU	C-N-CA	5.41	124.86	119.24
1	B	148	MET	N-CA-C	5.36	117.97	109.50
1	B	181	ILE	CB-CA-C	-5.05	108.90	113.70

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	2956	0	2967	71	0
1	B	2956	0	2967	74	0
2	A	43	0	30	5	0
2	B	43	0	30	6	0
3	A	29	0	16	7	0
3	B	29	0	16	10	0
4	A	5	0	0	0	0
4	B	3	0	0	0	0
All	All	6064	0	6026	154	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 (154) 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:21:VAL:HG13	1:B:24:ALA:HB3	1.43	1.00
1:A:21:VAL:HG13	1:A:24:ALA:HB3	1.53	0.89
1:B:231:ARG:HD3	3:B:502:PKJ:H9	1.53	0.89
3:A:502:PKJ:H7	3:A:502:PKJ:O1	1.71	0.89
1:B:63:ASN:O	1:B:65:LEU:HD12	1.74	0.88
1:B:315:SER:HB3	1:B:318:GLU:HG2	1.62	0.80
1:A:318:GLU:HA	1:A:318:GLU:OE1	1.82	0.79
1:A:29:GLN:O	1:A:78:LEU:HD22	1.84	0.77
2:A:501:HEM:HHA	2:A:501:HEM:HBA2	1.67	0.74
3:B:502:PKJ:O1	3:B:502:PKJ:H5	1.86	0.73
1:A:217:ILE:HG21	1:A:349:ILE:HD11	1.70	0.72
1:B:27:ASN:O	1:B:74:LYS:HE2	1.93	0.69
1:A:282:THR:HG21	1:B:297:ARG:NE	2.08	0.69
1:B:315:SER:CB	1:B:318:GLU:HG2	2.22	0.69
1:A:282:THR:HA	1:A:289:ALA:HB1	1.75	0.67
1:A:217:ILE:HG21	1:A:349:ILE:CD1	2.24	0.67
2:A:501:HEM:HBB2	2:A:501:HEM:HMB2	1.76	0.67
2:B:501:HEM:HHA	2:B:501:HEM:HBA2	1.78	0.66
1:A:282:THR:HG21	1:B:297:ARG:HE	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:LEU:O	1:B:245:ASP:N	2.29	0.65
1:B:21:VAL:CG1	1:B:24:ALA:HB3	2.25	0.63
1:B:188:MET:HE3	1:B:319:PHE:HB2	1.80	0.63
1:A:280:GLN:HE21	1:A:280:GLN:HA	1.64	0.63
1:B:297:ARG:HH11	1:B:297:ARG:HG3	1.64	0.62
3:B:502:PKJ:C28	3:B:502:PKJ:S14	2.88	0.62
1:B:73:HIS:HA	1:B:76:GLN:HE21	1.64	0.61
1:B:180:VAL:HG11	1:B:202:GLU:HG2	1.82	0.61
1:A:231:ARG:HB2	3:A:502:PKJ:H10	1.82	0.60
1:A:25:LEU:HD12	1:A:26:PRO:HD2	1.83	0.60
2:B:501:HEM:C1C	3:B:502:PKJ:S19	2.95	0.59
1:A:281:GLN:HA	1:A:281:GLN:OE1	2.01	0.59
1:B:127:ALA:HA	1:B:131:LEU:HD12	1.85	0.59
1:B:279:ILE:O	1:B:281:GLN:N	2.36	0.59
1:A:293:GLN:HG2	1:B:297:ARG:HH12	1.70	0.57
1:B:180:VAL:HG21	1:B:203:ILE:HG13	1.88	0.56
2:B:501:HEM:HBA2	2:B:501:HEM:CHA	2.36	0.56
1:B:231:ARG:HD3	3:B:502:PKJ:C9	2.31	0.55
1:B:218:HIS:HA	1:B:353:TYR:HH	1.72	0.55
1:B:301:PRO:HA	1:B:304:ARG:HG2	1.89	0.54
1:A:178:ILE:HD13	1:A:273:PHE:CZ	2.42	0.54
1:A:395:THR:O	1:A:398:SER:HB2	2.07	0.54
1:A:40:MET:HE3	1:A:44:LYS:HE3	1.89	0.54
1:B:197:LEU:HD12	1:B:328:LEU:HA	1.89	0.54
1:A:177:ALA:HB2	1:A:206:CYS:HB2	1.90	0.53
1:A:105:ARG:HB2	1:A:250:GLU:HG2	1.91	0.53
1:A:88:MET:HE1	1:A:123:ILE:HG13	1.92	0.52
1:A:280:GLN:HA	1:A:280:GLN:NE2	2.24	0.52
3:A:502:PKJ:O1	3:A:502:PKJ:C12	2.43	0.52
1:B:32:LEU:HD21	1:B:78:LEU:HG	1.92	0.52
1:A:393:SER:O	1:A:397:LYS:HG2	2.11	0.51
1:A:277:LEU:HB2	1:A:279:ILE:HD12	1.92	0.51
1:B:181:ILE:HD13	1:B:276:LEU:HD13	1.91	0.51
1:A:24:ALA:HA	1:A:131:LEU:HB3	1.92	0.51
3:B:502:PKJ:O1	3:B:502:PKJ:C5	2.51	0.51
1:A:121:PRO:HG2	1:A:298:TYR:CD2	2.46	0.51
1:B:218:HIS:HA	1:B:353:TYR:OH	2.11	0.51
1:B:247:LEU:O	1:B:256:PRO:HA	2.11	0.51
1:A:43:ALA:HB2	1:A:82:VAL:HG13	1.92	0.51
1:A:354:ILE:HG12	3:A:502:PKJ:H9	1.93	0.51
1:A:34:ASP:C	1:A:36:TYR:H	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ASN:O	1:B:74:LYS:CE	2.58	0.51
1:A:231:ARG:HB2	3:A:502:PKJ:C9	2.42	0.50
1:A:180:VAL:HG21	1:A:203:ILE:HG13	1.92	0.50
1:A:177:ALA:O	1:A:180:VAL:HG22	2.11	0.50
1:B:188:MET:SD	1:B:316:VAL:HG22	2.52	0.49
1:A:319:PHE:O	1:A:323:LYS:HG2	2.13	0.49
1:B:56:ARG:NH2	1:B:98:ASP:O	2.43	0.49
1:B:180:VAL:CG2	1:B:203:ILE:HG13	2.41	0.49
1:A:14:GLU:N	1:A:14:GLU:CD	2.70	0.49
1:A:144:THR:O	1:A:145:TYR:C	2.56	0.49
2:A:501:HEM:NA	3:A:502:PKJ:N16	2.61	0.49
1:A:277:LEU:HB2	1:A:279:ILE:CD1	2.43	0.48
1:A:253:TRP:C	1:A:255:ASP:H	2.20	0.48
1:B:146:GLU:H	1:B:146:GLU:CD	2.21	0.48
1:B:274:ASP:OD2	1:B:281:GLN:HG2	2.13	0.48
1:A:264:ALA:HB2	3:A:502:PKJ:C18	2.44	0.48
1:B:359:SER:C	1:B:360:GLN:HG3	2.38	0.48
1:A:144:THR:O	1:A:148:MET:HG3	2.14	0.48
1:B:245:ASP:O	1:B:256:PRO:HB2	2.14	0.48
1:A:293:GLN:HG2	1:B:297:ARG:NH1	2.29	0.47
1:B:167:SER:OG	3:B:502:PKJ:S19	2.71	0.47
1:B:170:VAL:HG23	1:B:213:VAL:HG12	1.96	0.47
1:A:34:ASP:C	1:A:36:TYR:N	2.71	0.47
1:B:104:PRO:HB2	1:B:107:ILE:HG22	1.96	0.47
1:A:218:HIS:ND1	1:A:352:LYS:NZ	2.58	0.47
1:B:88:MET:HE2	1:B:124:LEU:HB3	1.96	0.47
1:B:318:GLU:OE1	1:B:318:GLU:HA	2.14	0.47
1:B:321:LEU:HD21	1:B:400:LEU:HD22	1.97	0.47
1:A:107:ILE:HD13	1:A:107:ILE:HA	1.73	0.47
1:B:356:ILE:O	1:B:359:SER:N	2.44	0.47
1:A:79:ALA:HB3	1:A:114:LEU:HD21	1.98	0.46
1:A:181:ILE:HB	1:A:182:PRO:HD3	1.97	0.46
1:A:297:ARG:NH2	1:B:290:GLN:HG3	2.30	0.46
1:B:264:ALA:HB2	3:B:502:PKJ:C18	2.45	0.46
1:B:356:ILE:O	1:B:357:PRO:C	2.58	0.46
1:A:25:LEU:HD12	1:A:25:LEU:HA	1.63	0.46
1:B:44:LYS:HA	1:B:44:LYS:HD2	1.74	0.46
1:B:321:LEU:HA	1:B:321:LEU:HD23	1.55	0.46
1:B:52:SER:O	1:B:54:GLN:N	2.49	0.46
1:A:34:ASP:O	1:A:36:TYR:N	2.49	0.46
1:B:264:ALA:HB3	2:B:501:HEM:C4D	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:VAL:HG22	1:A:248:VAL:HB	1.99	0.45
1:A:222:ASN:HA	1:A:223:PRO:HD2	1.83	0.45
1:A:180:VAL:CG2	1:A:203:ILE:HG13	2.46	0.45
1:B:76:GLN:HB3	1:B:114:LEU:HD11	1.98	0.45
1:B:272:CYS:HB3	1:B:307:LEU:HD21	1.99	0.45
1:B:178:ILE:HD13	1:B:273:PHE:CZ	2.52	0.44
1:B:388:LEU:HD23	1:B:388:LEU:HA	1.84	0.44
1:B:33:PRO:HG2	1:B:36:TYR:CD2	2.52	0.44
1:A:123:ILE:HG12	1:A:124:LEU:N	2.33	0.44
1:A:269:VAL:HG12	1:A:270:PHE:CD1	2.53	0.44
1:A:237:TRP:HB3	1:A:243:LEU:HD12	1.99	0.44
1:A:301:PRO:O	1:A:302:ALA:C	2.61	0.44
1:B:297:ARG:HG3	1:B:297:ARG:NH1	2.31	0.43
1:B:46:LEU:O	1:B:50:ILE:HD12	2.18	0.43
1:A:30:GLU:H	1:A:30:GLU:HG2	1.71	0.43
1:A:46:LEU:N	1:A:47:PRO:CD	2.82	0.43
1:A:148:MET:HB2	1:A:165:LEU:HD21	1.99	0.43
1:A:297:ARG:HH22	1:B:290:GLN:HG3	1.84	0.43
1:B:240:ASN:HA	1:B:241:PRO:HD2	1.81	0.43
1:B:294:ASP:OD1	1:B:294:ASP:N	2.51	0.43
1:B:307:LEU:HD23	1:B:307:LEU:HA	1.78	0.43
2:B:501:HEM:NC	3:B:502:PKJ:S19	2.92	0.43
1:A:23:PHE:HD2	1:A:269:VAL:HG23	1.83	0.42
1:A:67:ILE:HB	1:A:70:LEU:HD12	2.00	0.42
1:B:33:PRO:HG2	1:B:36:TYR:CE2	2.54	0.42
1:A:247:LEU:O	1:A:256:PRO:HA	2.19	0.42
1:B:298:TYR:CD1	1:B:298:TYR:N	2.88	0.42
1:B:191:GLN:HG3	1:B:191:GLN:O	2.19	0.42
1:B:217:ILE:HD13	1:B:217:ILE:HA	1.86	0.42
1:B:176:SER:HB2	1:B:206:CYS:SG	2.58	0.42
1:B:43:ALA:HA	1:B:46:LEU:HD13	2.00	0.42
1:A:103:LEU:O	1:A:104:PRO:C	2.60	0.41
1:A:359:SER:O	1:A:360:GLN:HB3	2.20	0.41
1:B:196:LEU:HD23	1:B:328:LEU:HD11	2.01	0.41
1:B:18:ASP:OD1	1:B:20:GLU:N	2.46	0.41
1:B:32:LEU:HG	1:B:40:MET:CE	2.51	0.41
1:A:106:ASN:OD1	1:A:106:ASN:N	2.52	0.41
1:A:212:GLN:HA	1:A:215:HIS:CD2	2.55	0.41
2:A:501:HEM:HBA2	2:A:501:HEM:CHA	2.38	0.41
1:B:124:LEU:HD11	1:B:129:CYS:HB3	2.01	0.41
1:B:400:LEU:HD23	1:B:400:LEU:HA	1.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:502:PKJ:S14	3:B:502:PKJ:H2	2.60	0.40
1:A:14:GLU:CD	1:A:14:GLU:H	2.29	0.40
1:A:27:ASN:H	1:A:74:LYS:NZ	2.18	0.40
1:B:52:SER:C	1:B:54:GLN:H	2.30	0.40
1:B:189:GLN:C	1:B:191:GLN:H	2.28	0.40
1:A:107:ILE:O	1:A:110:PRO:HD2	2.21	0.40
2:B:501:HEM:HBB2	2:B:501:HEM:CMB	2.51	0.40
1:A:36:TYR:O	1:A:39:TRP:HB2	2.21	0.40
1:A:59:VAL:O	1:A:62:LEU:HB2	2.22	0.40
1:A:264:ALA:HB3	2:A:501:HEM:C1D	2.56	0.40
1:A:339:LEU:HD23	1:A:339:LEU:HA	1.88	0.40
1:B:228:SER:OG	1:B:229:VAL:HG23	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	369/423 (87%)	340 (92%)	28 (8%)	1 (0%)	36	66
1	B	369/423 (87%)	339 (92%)	25 (7%)	5 (1%)	9	30
All	All	738/846 (87%)	679 (92%)	53 (7%)	6 (1%)	16	44

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	244	SER
1	A	35	PHE
1	B	143	LEU
1	B	280	GLN
1	B	285	GLY
1	B	53	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	322/365 (88%)	300 (93%)	22 (7%)	14	42
1	B	322/365 (88%)	292 (91%)	30 (9%)	8	27
All	All	644/730 (88%)	592 (92%)	52 (8%)	11	33

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	21	VAL
1	A	55	LEU
1	A	57	GLU
1	A	58	ARG
1	A	61	LYS
1	A	107	ILE
1	A	165	LEU
1	A	176	SER
1	A	192	GLU
1	A	197	LEU
1	A	214	PHE
1	A	222	ASN
1	A	237	TRP
1	A	245	ASP
1	A	269	VAL
1	A	272	CYS
1	A	281	GLN
1	A	318	GLU
1	A	349	ILE
1	A	360	GLN
1	A	401	LYS
1	B	12	SER
1	B	13	LYS
1	B	21	VAL
1	B	46	LEU
1	B	54	GLN

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Mol	Chain	Res	Type
1	B	55	LEU
1	B	57	GLU
1	B	60	GLU
1	B	61	LYS
1	B	82	VAL
1	B	106	ASN
1	B	107	ILE
1	B	116	LYS
1	B	125	VAL
1	B	153	SER
1	B	155	ARG
1	B	180	VAL
1	B	181	ILE
1	B	197	LEU
1	B	214	PHE
1	B	217	ILE
1	B	222	ASN
1	B	237	TRP
1	B	272	CYS
1	B	290	GLN
1	B	294	ASP
1	B	309	SER
1	B	311	GLU
1	B	384	LEU
1	B	393	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	HIS
1	A	280	GLN
1	A	293	GLN
1	A	360	GLN
1	B	76	GLN
1	B	215	HIS
1	B	293	GLN
1	B	313	ASN

5.3.3 RNA ⓘ

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](#)

4 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$
3	PKJ	B	502	2	33,33,33	0.87	0	46,47,47	2.68	18 (39%)
3	PKJ	A	502	2	33,33,33	0.80	0	46,47,47	2.37	17 (36%)
2	HEM	A	501	1,3	50,50,50	1.63	10 (20%)	67,82,82	1.84	21 (31%)
2	HEM	B	501	1,3	50,50,50	1.49	6 (12%)	67,82,82	1.83	16 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PKJ	B	502	2	-	0/13/19/19	0/5/5/5
3	PKJ	A	502	2	-	0/13/19/19	0/5/5/5
2	HEM	A	501	1,3	-	7/14/54/54	-
2	HEM	B	501	1,3	-	7/14/54/54	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C4B-NB	-4.27	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	FE-NB	4.07	2.07	1.94
2	B	501	HEM	C1B-NB	-3.94	1.33	1.40
2	B	501	HEM	FE-NB	3.93	2.07	1.94
2	B	501	HEM	FE-NC	3.84	2.07	1.95
2	A	501	HEM	C1B-NB	-3.55	1.34	1.40
2	A	501	HEM	FE-NC	3.34	2.06	1.95
2	A	501	HEM	C1C-NC	-3.19	1.33	1.39
2	B	501	HEM	C4B-NB	-3.07	1.32	1.38
2	A	501	HEM	C4D-ND	-3.01	1.35	1.40
2	A	501	HEM	C1C-C2C	-2.93	1.39	1.45
2	B	501	HEM	C1D-ND	-2.55	1.33	1.38
2	A	501	HEM	C1D-C2D	2.14	1.48	1.44
2	A	501	HEM	FE-ND	-2.10	1.88	1.94
2	A	501	HEM	C1D-ND	-2.03	1.34	1.38
2	B	501	HEM	C4D-ND	-2.02	1.36	1.40

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	PKJ	C9-O10-C11	-6.20	97.01	105.32
3	B	502	PKJ	C21-N22-C18	5.98	117.93	114.28
3	A	502	PKJ	C21-N22-C18	5.62	117.71	114.28
2	B	501	HEM	CHC-C4B-NB	5.29	130.11	124.42
3	B	502	PKJ	C4-N3-C2	-5.15	118.40	127.52
3	A	502	PKJ	C9-O10-C11	-5.10	98.48	105.32
2	B	501	HEM	C1B-NB-C4B	5.04	111.17	105.21
3	B	502	PKJ	C13-C2-N3	-4.94	107.30	114.55
3	B	502	PKJ	C9-O8-C7	-4.93	98.71	105.32
3	A	502	PKJ	C13-C2-N3	-4.86	107.43	114.55
2	A	501	HEM	CHC-C4B-NB	4.72	129.50	124.42
3	A	502	PKJ	O10-C9-O8	4.53	115.20	108.09
3	A	502	PKJ	C4-N3-C2	-4.38	119.77	127.52
3	B	502	PKJ	O10-C9-O8	4.21	114.70	108.09
3	B	502	PKJ	S19-C18-N17	-4.16	135.96	139.17
2	B	501	HEM	C3B-C4B-NB	-4.14	106.49	109.47
2	A	501	HEM	CHA-C4D-ND	4.02	129.34	124.37
2	A	501	HEM	CHD-C1D-ND	4.00	128.73	124.42
2	A	501	HEM	C1B-NB-C4B	4.00	109.94	105.21
3	B	502	PKJ	N22-C18-N17	3.88	114.56	110.89
3	A	502	PKJ	C9-O8-C7	-3.88	100.12	105.32
3	A	502	PKJ	O10-C11-C7	3.84	114.44	109.79
3	B	502	PKJ	O10-C11-C7	3.83	114.42	109.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	PKJ	C4-C12-C11	-3.70	114.53	119.27
2	B	501	HEM	CHD-C4C-NC	3.55	128.32	124.45
3	A	502	PKJ	C5-C4-C12	3.48	123.86	119.66
3	B	502	PKJ	C5-C4-C12	3.47	123.84	119.66
3	B	502	PKJ	O1-C2-C13	3.46	127.30	121.44
3	B	502	PKJ	C13-S14-C15	-3.45	92.01	99.04
2	B	501	HEM	CHB-C1B-NB	3.42	128.60	124.37
2	A	501	HEM	CHB-C1B-NB	3.38	128.55	124.37
2	A	501	HEM	CHA-C4D-C3D	-3.32	119.11	125.23
3	A	502	PKJ	C4-C12-C11	-3.23	115.13	119.27
3	B	502	PKJ	O10-C11-C12	-3.20	123.60	127.86
2	A	501	HEM	CHD-C1D-C2D	-3.18	120.01	125.03
2	A	501	HEM	CMD-C2D-C1D	3.07	129.84	125.03
3	B	502	PKJ	C5-C6-C7	-3.06	114.27	120.06
3	A	502	PKJ	O10-C11-C12	-3.04	123.82	127.86
2	B	501	HEM	CHD-C1D-C2D	-3.04	120.23	125.03
2	B	501	HEM	CHA-C4D-ND	3.01	128.09	124.37
3	A	502	PKJ	C21-N22-C15	-2.97	138.20	141.94
3	A	502	PKJ	O1-C2-C13	2.96	126.46	121.44
2	B	501	HEM	CHA-C4D-C3D	-2.94	119.81	125.23
2	A	501	HEM	CAA-C2A-C1A	2.92	130.65	124.94
2	A	501	HEM	O2A-CGA-CBA	2.92	123.23	114.00
3	A	502	PKJ	S14-C15-N16	2.82	131.86	127.78
2	A	501	HEM	O2D-CGD-CBD	2.67	122.44	114.00
3	B	502	PKJ	C21-N22-C15	-2.66	138.60	141.94
2	B	501	HEM	CHD-C1D-ND	2.59	127.21	124.42
2	B	501	HEM	C1A-CHA-C4D	-2.55	120.25	126.25
3	A	502	PKJ	C5-C6-C7	-2.51	115.31	120.06
3	A	502	PKJ	C23-C21-C20	-2.47	121.89	126.01
2	B	501	HEM	O2D-CGD-CBD	2.47	121.81	114.00
2	A	501	HEM	CBD-CAD-C3D	-2.44	105.78	112.53
2	B	501	HEM	CHA-C1A-NA	2.43	128.26	123.86
2	B	501	HEM	O2A-CGA-CBA	2.42	121.63	114.00
2	A	501	HEM	CHD-C4C-NC	2.40	127.06	124.45
2	A	501	HEM	CAD-C3D-C4D	2.35	128.78	124.70
2	A	501	HEM	C4C-CHD-C1D	-2.30	121.13	126.02
2	B	501	HEM	C2D-C1D-ND	2.28	112.53	109.90
2	A	501	HEM	C4A-CHB-C1B	-2.20	121.07	126.25
3	B	502	PKJ	C20-C21-N22	-2.17	110.00	111.70
3	A	502	PKJ	C24-C25-C26	-2.16	118.88	121.37
3	B	502	PKJ	C6-C7-C11	2.14	124.15	121.50
2	A	501	HEM	O2D-CGD-O1D	-2.13	117.85	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CAA-C2A-C3A	-2.05	122.46	127.07
2	B	501	HEM	O2D-CGD-O1D	-2.04	118.08	123.33
3	A	502	PKJ	S14-C15-N22	-2.04	117.52	121.37
2	B	501	HEM	CAD-C3D-C4D	2.04	128.25	124.70
2	A	501	HEM	CHB-C4A-NA	2.02	127.52	123.86
2	A	501	HEM	O2A-CGA-O1A	-2.01	118.16	123.33
2	A	501	HEM	C4C-NC-C1C	2.00	109.08	105.82

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	HEM	C1A-C2A-CAA-CBA
2	B	501	HEM	C1A-C2A-CAA-CBA
2	B	501	HEM	C2C-C3C-CAC-CBC
2	A	501	HEM	C3A-C2A-CAA-CBA
2	B	501	HEM	C3A-C2A-CAA-CBA
2	A	501	HEM	C2C-C3C-CAC-CBC
2	B	501	HEM	C4C-C3C-CAC-CBC
2	B	501	HEM	C2A-CAA-CBA-CGA
2	A	501	HEM	C4C-C3C-CAC-CBC
2	A	501	HEM	C3D-CAD-CBD-CGD
2	B	501	HEM	CAD-CBD-CGD-O1D
2	A	501	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	CAA-CBA-CGA-O2A
2	B	501	HEM	CAD-CBD-CGD-O2D

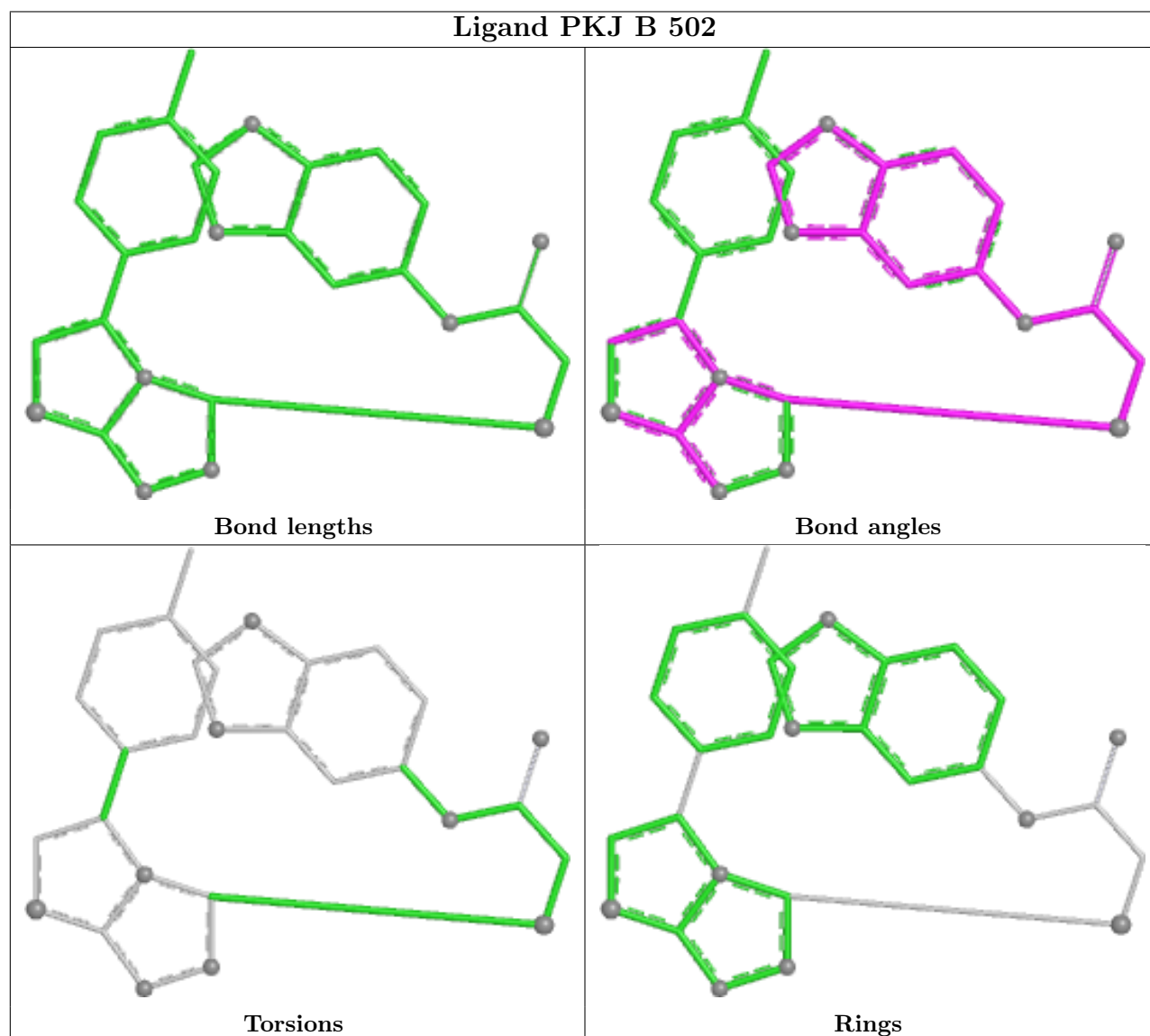
There are no ring outliers.

4 monomers are involved in 25 short contacts:

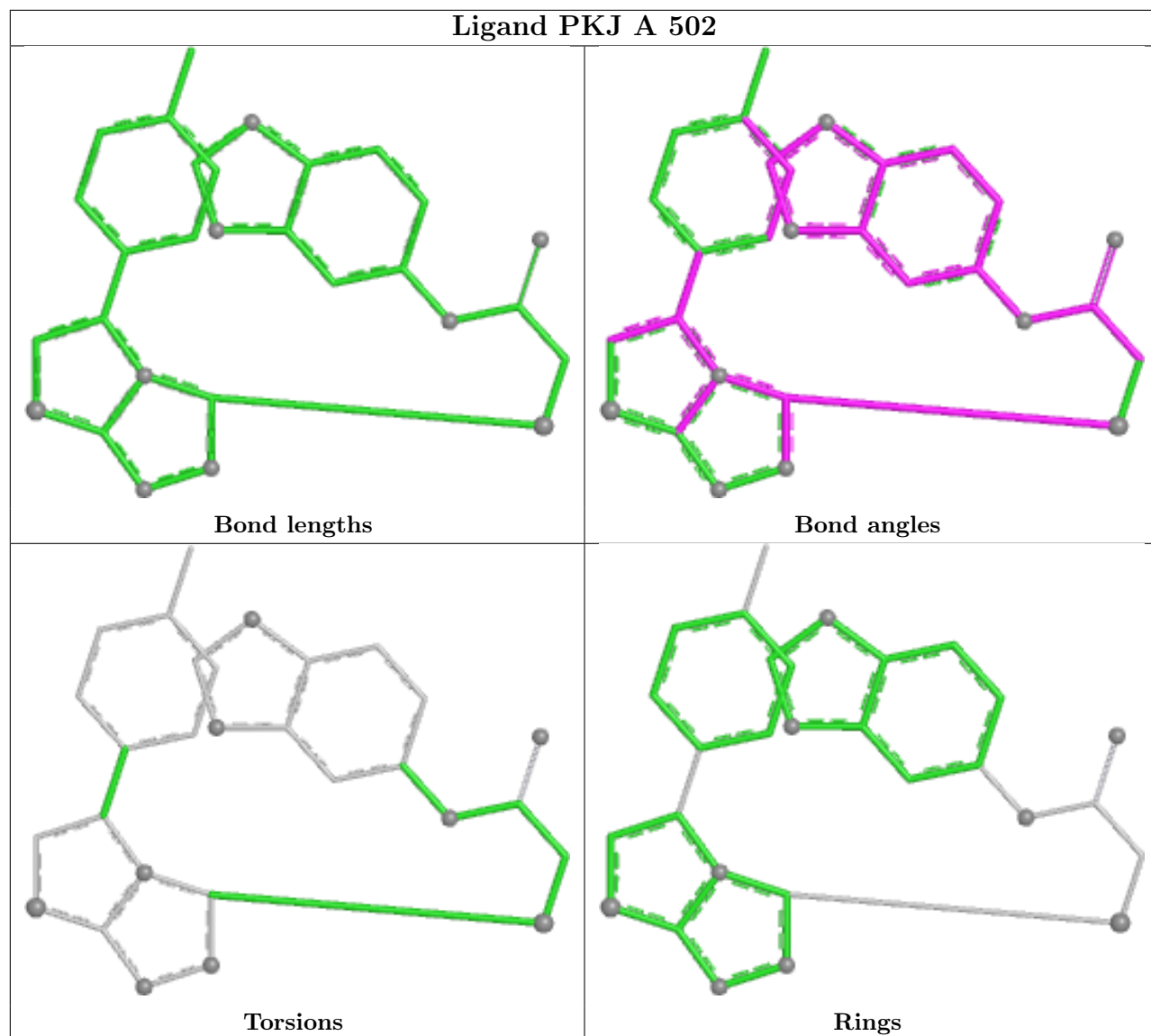
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	PKJ	10	0
3	A	502	PKJ	7	0
2	A	501	HEM	5	0
2	B	501	HEM	6	0

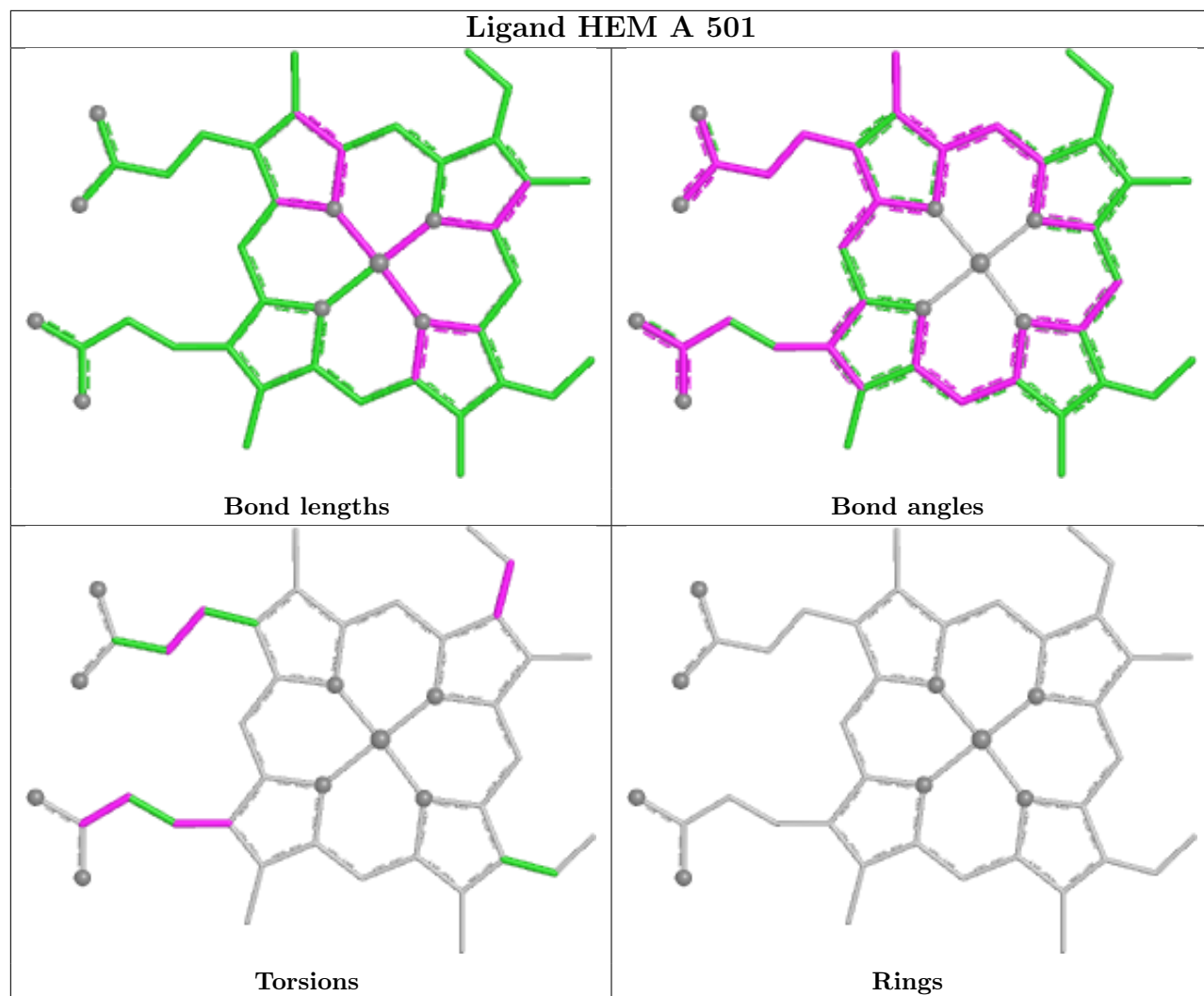
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

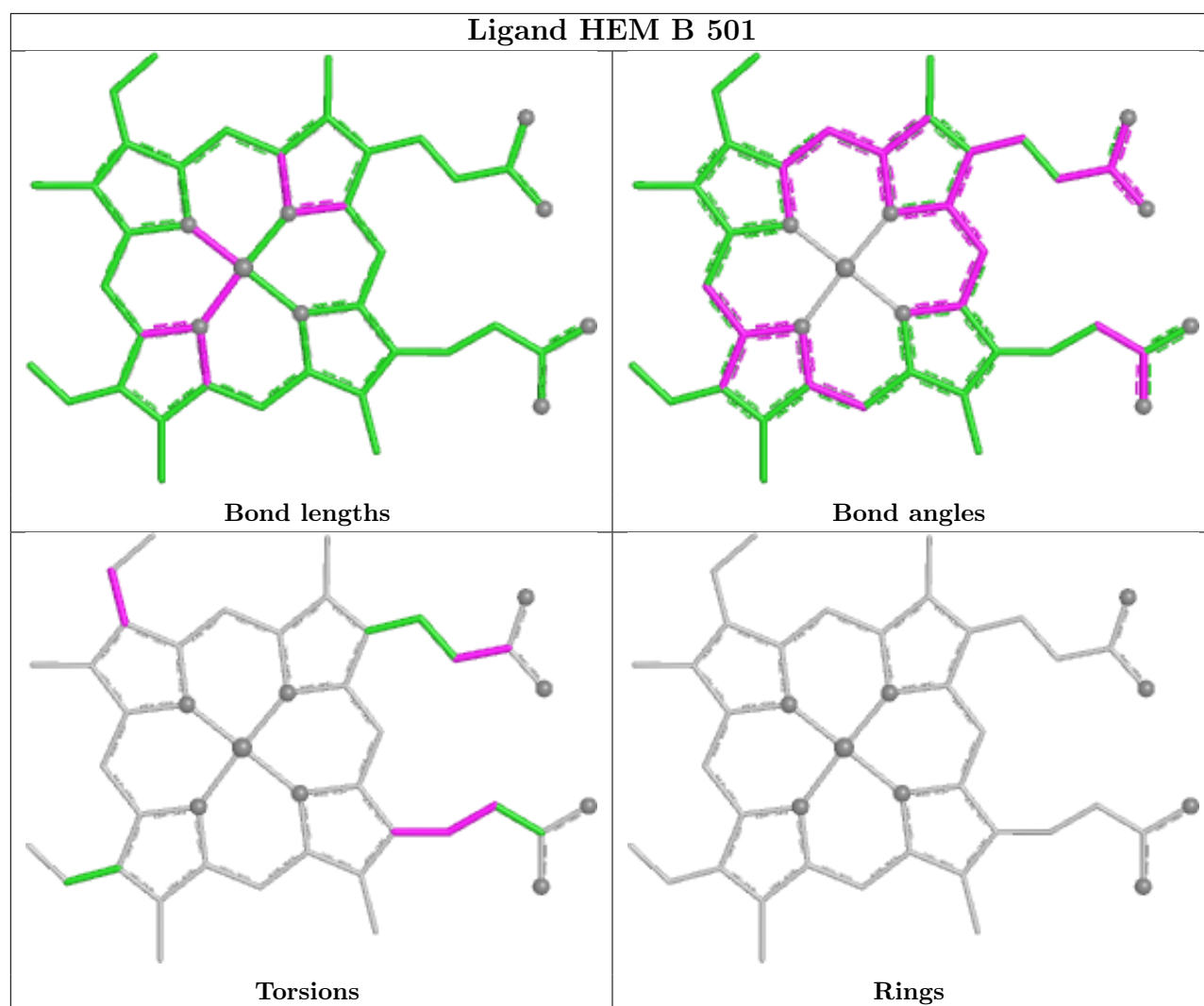
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



Ligand PKJ A 502







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	373/423 (88%)	-0.33	5 (1%) 75 66	26, 50, 87, 134	0
1	B	373/423 (88%)	-0.19	5 (1%) 75 66	36, 60, 99, 140	0
All	All	746/846 (88%)	-0.26	10 (1%) 75 66	26, 54, 94, 140	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283	ALA	5.3
1	A	284	GLY	4.1
1	B	380	GLY	3.1
1	A	380	GLY	3.0
1	B	12	SER	2.8
1	A	254	GLU	2.8
1	A	403	GLY	2.7
1	B	13	LYS	2.5
1	B	283	ALA	2.4
1	B	401	LYS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

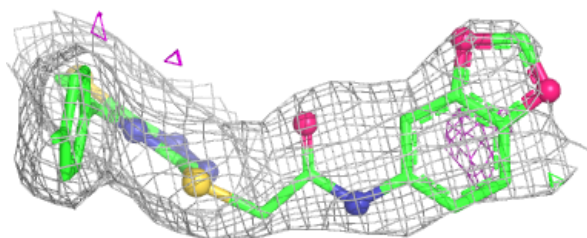
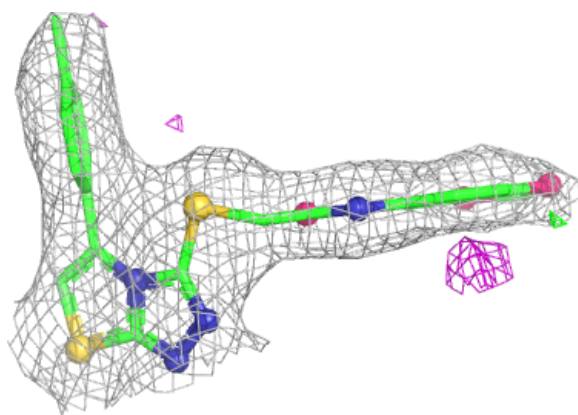
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PKJ	A	502	29/29	0.97	0.07	33,37,93,103	0
3	PKJ	B	502	29/29	0.97	0.08	35,43,96,108	0
2	HEM	B	501	43/43	0.98	0.07	35,39,53,71	0
2	HEM	A	501	43/43	0.99	0.06	26,32,47,52	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.

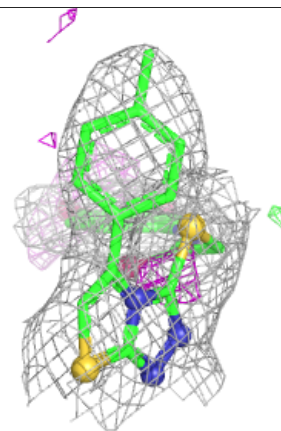
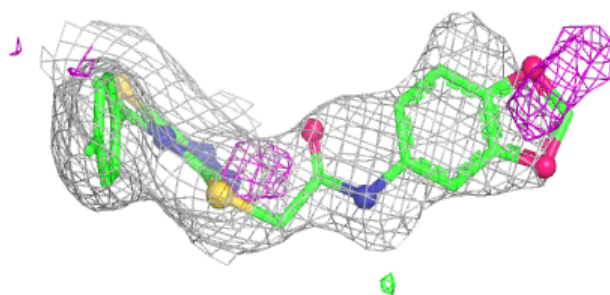
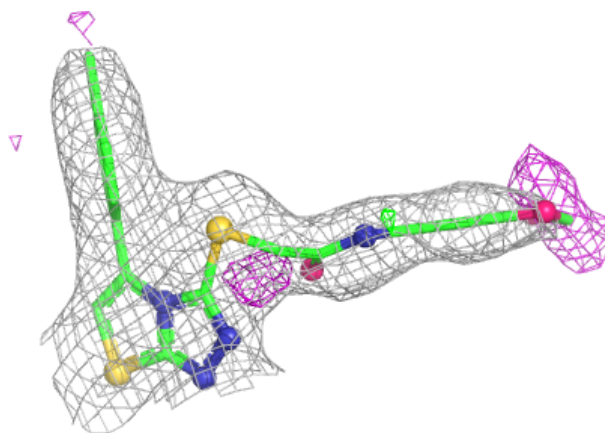
Electron density around PKJ A 502:

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



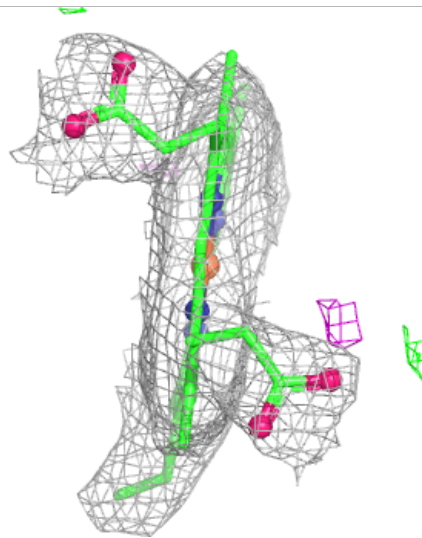
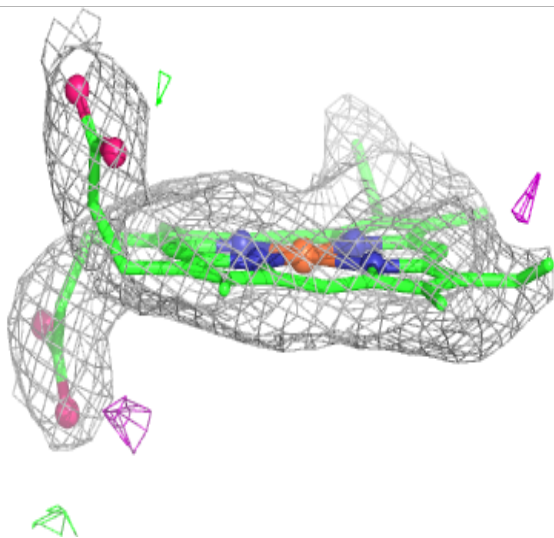
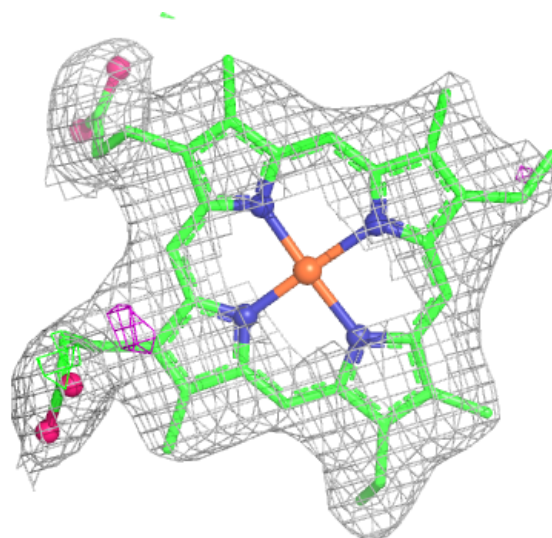
Electron density around PKJ B 502:

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



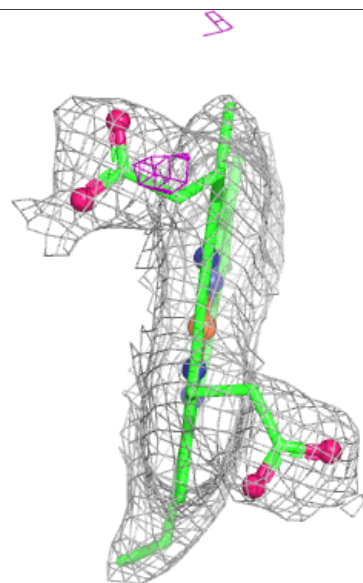
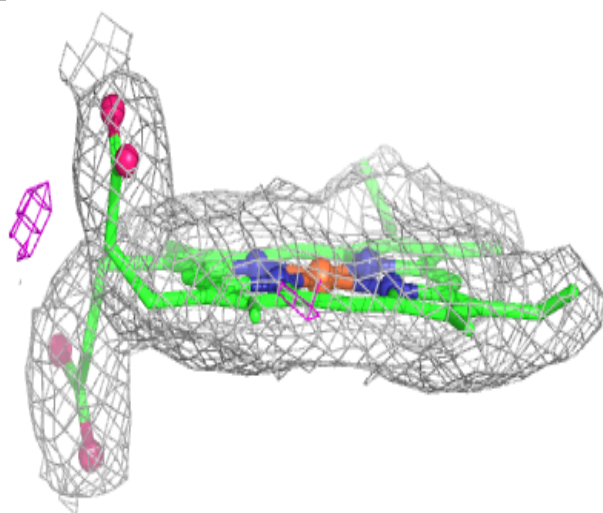
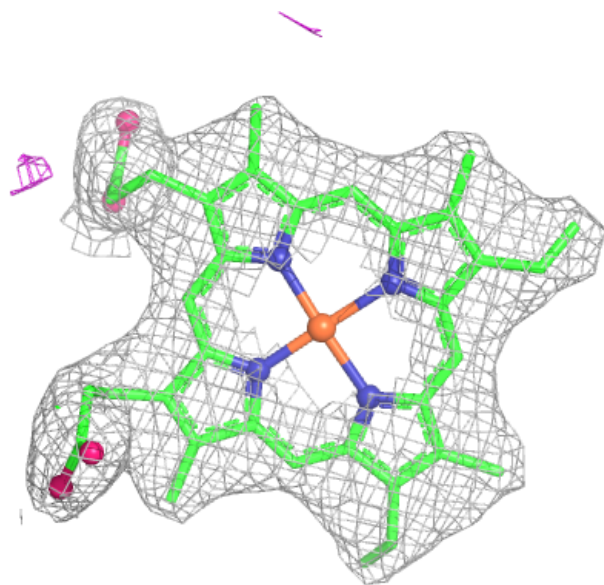
Electron density around HEM B 501:

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



Electron density around HEM A 501:

$2mF_o-DF_c$ (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.