



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:43 PM UTC

PDB ID : 2D0T / pdb_00002d0t
Title : Crystal structure of 4-phenylimidazole bound form of human indoleamine 2,3-dioxygenase
Authors : Sugimoto, H.; Oda, S.; Otsuki, T.; Hino, T.; Yoshida, T.; Shiro, Y.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-08-08
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

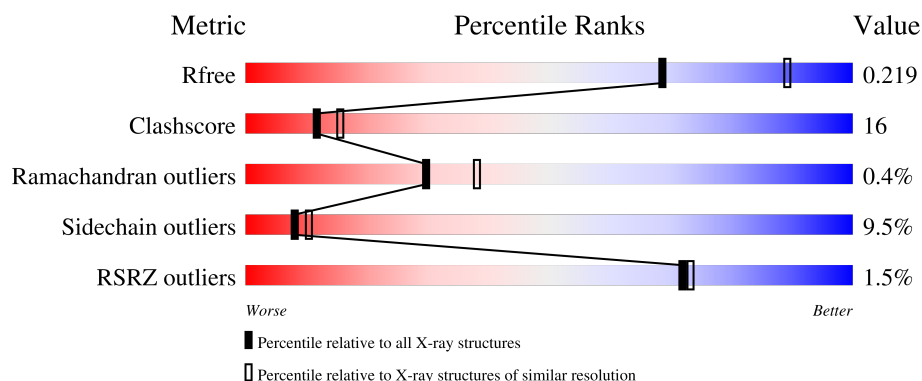
1 Overall quality at a glance

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	406	64% 24% 8%
1	B	406	62% 27% 8%

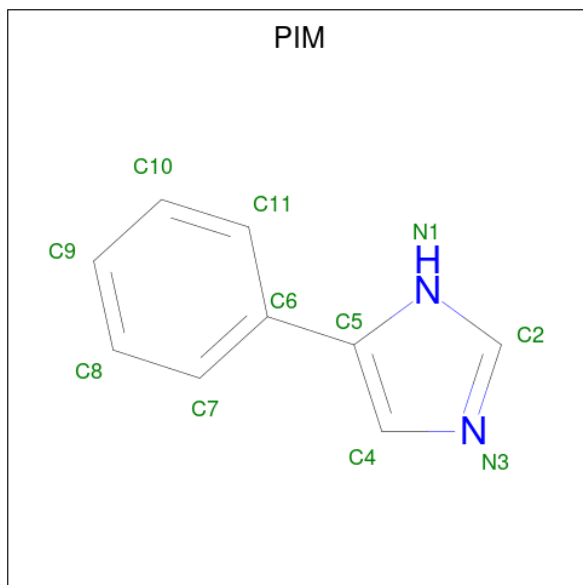
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NHE	A	503	-	-	X	-



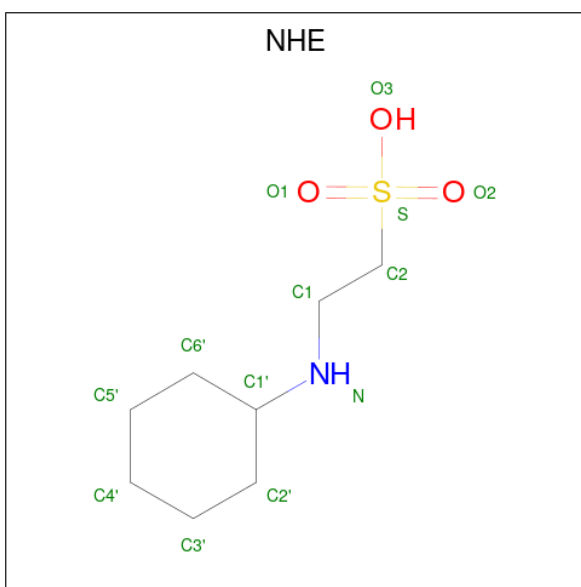
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 3 is 4-PHENYL-1H-IMIDAZOLE (CCD ID: PIM) (formula: C₉H₈N₂).



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

- Molecule 4 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (CCD ID: NHE) (formula: C₈H₁₇NO₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
4	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
4	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
4	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	72	Total	O	0	0
			72	72		
5	B	66	Total	O	0	0
			66	66		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.07Å 98.03Å 130.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.30 19.94 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.7 (19.94-2.30) 90.7 (19.94-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.30Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.191 , 0.221 0.187 , 0.219	Depositor DCC
R_{free} test set	2179 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	46.3	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6218	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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: PIM, NHE, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.55	1/3024 (0.0%)	1.00	18/4087 (0.4%)
1	B	0.51	0/3032	0.96	8/4098 (0.2%)
All	All	0.53	1/6056 (0.0%)	0.98	26/8185 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	181	ILE	CA-CB	5.92	1.57	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	THR	N-CA-C	8.75	120.59	111.14
1	A	265	GLY	N-CA-C	-7.60	106.31	114.67
1	B	71	THR	N-CA-C	7.24	120.24	111.40
1	B	265	GLY	N-CA-C	-6.93	107.04	114.67
1	B	15	TYR	N-CA-C	-6.91	103.97	112.88
1	B	315	SER	N-CA-C	6.87	120.19	109.96
1	A	401	LYS	N-CA-C	6.50	120.21	112.93
1	A	323	LYS	N-CA-C	6.48	123.13	114.12
1	A	382	THR	N-CA-C	-6.21	105.86	113.50
1	B	227	PHE	N-CA-C	6.13	118.04	111.36
1	A	309	SER	N-CA-C	-6.11	104.73	111.82
1	A	94	LYS	N-CA-C	-6.05	105.99	113.19
1	A	181	ILE	CB-CA-C	-6.03	107.98	113.70
1	A	269	VAL	N-CA-C	5.79	116.26	110.23
1	A	315	SER	N-CA-C	5.78	118.08	109.59
1	B	103	LEU	CA-C-N	5.53	125.85	119.93
1	B	103	LEU	C-N-CA	5.53	125.85	119.93
1	B	382	THR	N-CA-C	-5.46	106.78	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	ASP	N-CA-C	-5.32	105.56	111.36
1	A	167	SER	N-CA-C	-5.25	105.56	111.28
1	A	307	LEU	CA-C-N	-5.13	112.51	122.06
1	A	307	LEU	C-N-CA	-5.13	112.51	122.06
1	A	240	ASN	CA-C-N	5.09	124.53	119.24
1	A	240	ASN	C-N-CA	5.09	124.53	119.24
1	A	402	GLU	N-CA-C	5.05	116.86	111.36
1	A	107	ILE	N-CA-C	-5.00	107.85	111.90

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	89	1
1	B	2964	0	2978	96	1
2	A	43	0	30	6	0
2	B	43	0	30	5	0
3	A	11	0	8	2	0
3	B	11	0	8	2	0
4	A	26	0	32	8	0
4	B	26	0	33	5	0
5	A	72	0	0	5	0
5	B	66	0	0	4	0
All	All	6218	0	6086	193	1

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 16.

All (193) 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:A:401:LYS:HE2	1:A:401:LYS:HA	1.17	1.15
1:B:21:VAL:HG13	1:B:24:ALA:HB3	1.39	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:LYS:HD2	1:B:14:GLU:H	1.25	0.99
1:A:21:VAL:HG13	1:A:24:ALA:HB3	1.43	0.97
4:A:502:NHE:HC21	4:A:503:NHE:HN	1.31	0.95
1:B:105:ARG:HB3	1:B:250:GLU:HG2	1.57	0.86
1:A:401:LYS:HA	1:A:401:LYS:CE	2.06	0.83
1:A:329:ARG:HE	1:A:401:LYS:HD2	1.44	0.82
1:A:136:LYS:HE2	1:A:141:LYS:O	1.80	0.81
1:A:401:LYS:HE2	1:A:401:LYS:CA	2.02	0.81
1:A:188:MET:HG2	1:A:319:PHE:CD2	2.16	0.81
1:B:21:VAL:CG1	1:B:24:ALA:HB3	2.14	0.77
1:B:88:MET:HE3	1:B:233:TYR:O	1.84	0.77
1:A:385:MET:HA	1:A:385:MET:HE2	1.67	0.75
1:B:80:ARG:NH2	1:B:121:PRO:O	2.20	0.75
1:B:13:LYS:HD2	1:B:14:GLU:N	2.02	0.75
1:A:329:ARG:NE	1:A:401:LYS:HD2	2.01	0.74
1:A:102:VAL:HG22	1:A:248:VAL:HG11	1.70	0.71
1:B:109:VAL:O	1:B:113:GLN:HG3	1.90	0.71
1:B:88:MET:SD	5:B:1511:HOH:O	2.49	0.69
1:B:102:VAL:HG22	1:B:248:VAL:HG11	1.72	0.69
1:A:23:PHE:HD2	1:A:269:VAL:HG23	1.58	0.69
1:B:13:LYS:CD	1:B:14:GLU:H	2.04	0.67
4:A:503:NHE:C2	4:A:503:NHE:H6'1	2.25	0.67
1:A:255:ASP:HB3	1:A:256:PRO:HD2	1.78	0.66
1:B:255:ASP:HB3	1:B:256:PRO:HD2	1.76	0.66
1:A:125:VAL:HG13	5:A:504:HOH:O	1.94	0.66
1:A:32:LEU:HG	1:A:78:LEU:HD13	1.79	0.65
1:A:102:VAL:HG22	1:A:248:VAL:CG1	2.26	0.65
1:B:23:PHE:HD2	1:B:269:VAL:HG23	1.61	0.64
1:A:262:GLY:O	4:A:502:NHE:HC'1	1.97	0.64
1:A:14:GLU:C	1:A:16:HIS:H	2.05	0.64
1:B:102:VAL:HG22	1:B:248:VAL:CG1	2.27	0.64
1:A:347:LEU:HD12	1:A:392:ARG:HH11	1.63	0.64
1:B:262:GLY:O	4:B:1502:NHE:HC'1	1.98	0.63
1:A:181:ILE:HB	1:A:182:PRO:HD3	1.81	0.63
1:A:263:SER:HA	3:A:501:PIM:HN1	1.64	0.63
1:B:218:HIS:HD2	1:B:352:LYS:NZ	1.99	0.61
1:A:217:ILE:HG21	1:A:349:ILE:HD13	1.82	0.60
1:A:14:GLU:C	1:A:14:GLU:CD	2.69	0.60
1:B:401:LYS:O	1:B:402:GLU:HG2	2.02	0.59
1:B:83:LEU:HD22	1:B:107:ILE:HD11	1.83	0.59
1:A:217:ILE:O	1:A:217:ILE:HD13	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ALA:HB1	4:B:1502:NHE:O3	2.03	0.59
1:B:340:VAL:HG12	1:B:395:THR:HG22	1.85	0.58
1:B:102:VAL:HA	1:B:248:VAL:HG13	1.85	0.58
1:B:11:ILE:HG22	1:B:12:SER:N	2.19	0.58
2:B:404:HEM:HBA1	4:B:1503:NHE:H6'2	1.85	0.57
1:B:180:VAL:HG21	1:B:203:ILE:HG13	1.86	0.57
1:B:321:LEU:HD21	1:B:400:LEU:HD22	1.87	0.57
1:B:356:ILE:HB	1:B:357:PRO:HD3	1.86	0.57
1:B:401:LYS:HG2	1:B:402:GLU:N	2.20	0.56
1:A:347:LEU:HD12	1:A:392:ARG:NH1	2.19	0.56
1:B:402:GLU:O	1:B:402:GLU:HG3	2.04	0.56
4:A:503:NHE:H6'1	4:A:503:NHE:HC21	1.86	0.56
1:B:24:ALA:HA	1:B:131:LEU:HD22	1.87	0.55
1:A:146:GLU:H	1:A:146:GLU:CD	2.14	0.55
1:B:57:GLU:HG3	1:B:58:ARG:N	2.20	0.55
1:B:57:GLU:O	1:B:61:LYS:HG2	2.07	0.55
1:B:23:PHE:CD2	1:B:269:VAL:HG23	2.42	0.55
1:A:217:ILE:HG21	1:A:349:ILE:CD1	2.37	0.54
1:B:191:GLN:HE21	1:B:191:GLN:CA	2.19	0.54
1:B:115:SER:HB3	1:B:120:LEU:O	2.07	0.54
1:A:83:LEU:HD22	1:A:107:ILE:HD11	1.90	0.54
1:A:23:PHE:CD2	1:A:269:VAL:HG23	2.42	0.54
1:B:287:HIS:HE1	4:B:1503:NHE:H4'2	1.72	0.54
1:B:287:HIS:CE1	4:B:1503:NHE:H4'2	2.42	0.54
1:A:109:VAL:HB	1:A:110:PRO:HD3	1.89	0.53
1:A:305:ASN:CG	1:B:312:SER:HB2	2.33	0.53
1:A:401:LYS:CE	1:A:401:LYS:CA	2.78	0.53
1:B:384:LEU:HD11	2:B:404:HEM:HMA3	1.90	0.53
1:A:350:VAL:HG11	1:A:385:MET:CE	2.39	0.53
1:A:136:LYS:CE	1:A:141:LYS:O	2.53	0.53
1:A:384:LEU:HD22	4:A:503:NHE:O3	2.09	0.53
1:A:384:LEU:HD11	2:A:404:HEM:HMA3	1.91	0.52
1:B:52:SER:OG	1:B:54:GLN:HG3	2.09	0.52
1:B:13:LYS:CD	1:B:14:GLU:N	2.68	0.52
1:B:80:ARG:NH1	1:B:128:ASP:OD2	2.42	0.52
1:A:216:GLN:NE2	5:A:545:HOH:O	2.42	0.52
1:B:401:LYS:HG2	1:B:402:GLU:H	1.73	0.52
1:A:102:VAL:HA	1:A:248:VAL:HG13	1.90	0.52
1:B:266:GLN:O	1:B:299:MET:HG2	2.10	0.52
1:B:14:GLU:N	1:B:14:GLU:CD	2.68	0.51
1:A:222:ASN:ND2	5:A:528:HOH:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:LEU:HD22	1:B:107:ILE:CD1	2.41	0.51
1:B:214:PHE:HD1	1:B:214:PHE:O	1.94	0.51
1:A:350:VAL:HG11	1:A:385:MET:HE1	1.92	0.51
1:B:191:GLN:NE2	1:B:191:GLN:HA	2.26	0.51
1:B:253:TRP:CE3	1:B:257:LYS:HG3	2.46	0.51
1:A:55:LEU:CD2	1:A:89:ALA:HB1	2.41	0.50
1:B:218:HIS:HD2	1:B:352:LYS:HZ3	1.58	0.50
1:A:115:SER:HB3	1:A:120:LEU:O	2.10	0.50
1:B:336:VAL:O	1:B:340:VAL:HG13	2.12	0.50
1:A:109:VAL:O	1:A:113:GLN:HG3	2.12	0.50
1:A:205:SER:O	1:A:209:LYS:HG3	2.12	0.49
1:A:50:ILE:HG12	1:A:55:LEU:HD22	1.95	0.49
1:A:340:VAL:HG12	1:A:395:THR:HG22	1.93	0.49
1:A:101:LYS:O	1:A:248:VAL:HG12	2.13	0.49
1:B:317:ARG:HD2	1:B:332:TYR:OH	2.11	0.49
1:A:188:MET:HG2	1:A:319:PHE:CE2	2.46	0.49
1:B:88:MET:HG2	5:B:1511:HOH:O	2.13	0.48
1:B:217:ILE:HG21	1:B:349:ILE:HD12	1.94	0.48
1:A:25:LEU:HD23	1:A:28:PRO:HB3	1.95	0.48
1:A:29:GLN:O	1:A:78:LEU:HG	2.14	0.48
1:B:155:ARG:HD2	1:B:233:TYR:OH	2.13	0.48
1:A:28:PRO:HG2	1:A:134:TRP:O	2.14	0.48
1:A:347:LEU:CD1	1:A:392:ARG:HH11	2.25	0.48
1:B:191:GLN:HE21	1:B:191:GLN:HA	1.79	0.48
1:B:385:MET:HA	1:B:385:MET:HE2	1.94	0.48
1:B:43:ALA:HB2	1:B:82:VAL:HG13	1.95	0.48
1:B:301:PRO:HA	1:B:304:ARG:NH1	2.28	0.48
1:A:347:LEU:CD1	1:A:392:ARG:NH1	2.76	0.47
1:B:125:VAL:HG13	5:B:1506:HOH:O	2.14	0.47
1:A:24:ALA:HA	1:A:131:LEU:HD22	1.97	0.47
1:B:121:PRO:HG3	1:B:298:TYR:CD2	2.50	0.47
1:A:356:ILE:HB	1:A:357:PRO:HD3	1.96	0.47
1:A:83:LEU:HD22	1:A:107:ILE:CD1	2.45	0.47
1:A:21:VAL:CG1	1:A:24:ALA:HB3	2.29	0.47
1:B:350:VAL:HG11	1:B:385:MET:CE	2.45	0.46
1:A:264:ALA:O	1:A:267:SER:HB3	2.15	0.46
1:B:263:SER:HA	3:B:1501:PIM:HN1	1.80	0.46
1:B:125:VAL:HG13	1:B:127:ALA:H	1.80	0.46
1:A:50:ILE:HD11	1:A:89:ALA:HB1	1.96	0.46
1:B:13:LYS:NZ	1:B:14:GLU:HB2	2.30	0.46
1:A:13:LYS:HB3	1:A:13:LYS:NZ	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:LEU:HD11	2:B:404:HEM:CMA	2.45	0.46
1:A:14:GLU:C	1:A:16:HIS:N	2.70	0.46
1:A:177:ALA:O	1:A:180:VAL:HG13	2.16	0.45
2:A:404:HEM:HBA1	4:A:503:NHE:H6'2	1.99	0.45
1:B:355:LEU:HD11	1:B:385:MET:SD	2.57	0.45
1:B:384:LEU:HD21	2:B:404:HEM:HMA3	1.98	0.45
1:A:102:VAL:HA	1:A:248:VAL:CG1	2.46	0.45
1:A:384:LEU:HD11	2:A:404:HEM:CMA	2.47	0.45
1:A:329:ARG:HE	1:A:401:LYS:CD	2.23	0.45
1:B:177:ALA:HB3	1:B:273:PHE:HZ	1.82	0.45
1:A:380:GLY:C	1:A:382:THR:H	2.24	0.44
1:B:125:VAL:CG2	1:B:298:TYR:HB3	2.47	0.44
1:A:80:ARG:HG3	1:A:118:LEU:HD12	1.99	0.44
1:A:146:GLU:CD	1:A:146:GLU:N	2.75	0.44
1:A:52:SER:OG	1:A:54:GLN:HG2	2.17	0.44
1:B:32:LEU:HG	1:B:78:LEU:HD13	2.00	0.44
1:A:100:ARG:HD3	1:A:100:ARG:HA	1.85	0.44
2:A:404:HEM:O2A	4:A:503:NHE:H6'2	2.18	0.44
1:B:333:ASP:O	1:B:337:LYS:HB2	2.18	0.44
1:B:218:HIS:CD2	1:B:352:LYS:NZ	2.84	0.44
1:A:63:ASN:O	1:A:65:LEU:HD13	2.18	0.44
1:A:93:GLY:C	1:A:95:GLY:H	2.26	0.44
1:B:101:LYS:O	1:B:248:VAL:HG12	2.19	0.43
1:A:297:ARG:NH2	5:A:575:HOH:O	2.50	0.43
1:B:197:LEU:HD12	1:B:331:ALA:HB2	2.00	0.43
1:B:11:ILE:CG2	1:B:12:SER:N	2.82	0.43
1:B:276:LEU:C	1:B:276:LEU:HD13	2.44	0.43
1:A:14:GLU:OE1	1:A:14:GLU:N	2.52	0.43
1:B:63:ASN:O	1:B:65:LEU:HD13	2.19	0.43
1:B:100:ARG:HA	1:B:100:ARG:HD3	1.80	0.43
1:A:147:ASN:O	1:A:147:ASN:CG	2.61	0.43
1:B:109:VAL:HB	1:B:110:PRO:HD3	2.00	0.43
1:A:196:LEU:HD12	1:A:319:PHE:CE2	2.54	0.42
1:A:50:ILE:CG1	1:A:55:LEU:HD22	2.49	0.42
1:B:221:VAL:HG12	1:B:353:TYR:CE2	2.55	0.42
1:A:214:PHE:CE1	1:A:349:ILE:HD12	2.55	0.42
2:A:404:HEM:C1A	3:A:501:PIM:H2	2.55	0.42
1:B:221:VAL:HG12	1:B:353:TYR:HE2	1.84	0.42
1:B:101:LYS:HG2	1:B:243:LEU:HD23	2.01	0.42
1:A:264:ALA:HB3	2:A:404:HEM:C1D	2.55	0.42
1:B:181:ILE:HB	1:B:182:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:VAL:CG1	1:A:385:MET:HE1	2.50	0.42
1:B:99:VAL:CG2	1:B:100:ARG:N	2.82	0.42
1:B:340:VAL:HG12	1:B:395:THR:CG2	2.50	0.42
2:B:404:HEM:C1A	3:B:1501:PIM:H2	2.55	0.42
1:A:80:ARG:NH2	1:A:128:ASP:OD2	2.53	0.41
1:B:88:MET:CG	5:B:1511:HOH:O	2.68	0.41
1:B:227:PHE:O	1:B:231:ARG:NH1	2.53	0.41
1:B:401:LYS:CG	1:B:402:GLU:H	2.32	0.41
4:A:503:NHE:H6'1	4:A:503:NHE:HC22	1.99	0.41
1:B:347:LEU:HD21	1:B:388:LEU:CB	2.50	0.41
1:B:226:PHE:CD2	1:B:226:PHE:C	2.99	0.41
1:B:401:LYS:CG	1:B:402:GLU:N	2.83	0.41
1:A:56:ARG:CZ	1:A:100:ARG:HG2	2.51	0.41
1:B:18:ASP:HB2	1:B:26:PRO:HG3	2.02	0.41
1:A:158:ASP:O	1:A:159:CYS:HB2	2.21	0.41
1:A:185:PHE:CE1	1:A:313:ASN:HB3	2.55	0.41
1:A:298:TYR:N	1:A:298:TYR:CD1	2.89	0.41
1:A:230:LEU:HD23	1:A:230:LEU:HA	1.82	0.41
1:B:102:VAL:HA	1:B:248:VAL:CG1	2.50	0.41
1:B:347:LEU:HD23	1:B:347:LEU:HA	1.78	0.41
1:A:196:LEU:HD12	1:A:319:PHE:HE2	1.86	0.40
1:B:55:LEU:HD22	1:B:89:ALA:HB1	2.03	0.40
1:B:291:PHE:CE1	1:B:295:MET:HE3	2.56	0.40
1:A:55:LEU:HD22	1:A:89:ALA:HB1	2.03	0.40
1:A:295:MET:HA	1:A:295:MET:HE2	2.03	0.40
1:A:95:GLY:HA2	5:A:525:HOH:O	2.21	0.40
1:B:296:ARG:HA	1:B:299:MET:HE3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:LYS:N	1:B:403:GLY:OXT[3_655]	2.02	0.18

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	369/406 (91%)	353 (96%)	14 (4%)	2 (0%)	24	31
1	B	370/406 (91%)	355 (96%)	14 (4%)	1 (0%)	36	46
All	All	739/812 (91%)	708 (96%)	28 (4%)	3 (0%)	30	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	244	SER
1	B	244	SER

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	322/350 (92%)	289 (90%)	33 (10%)	7	8
1	B	323/350 (92%)	295 (91%)	28 (9%)	9	12
All	All	645/700 (92%)	584 (90%)	61 (10%)	8	10

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	20	GLU
1	A	21	VAL
1	A	34	ASP
1	A	46	LEU
1	A	48	ASP
1	A	57	GLU
1	A	61	LYS
1	A	78	LEU

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Mol	Chain	Res	Type
1	A	99	VAL
1	A	105	ARG
1	A	107	ILE
1	A	125	VAL
1	A	144	THR
1	A	155	ARG
1	A	168	LEU
1	A	180	VAL
1	A	181	ILE
1	A	186	LYS
1	A	190	MET
1	A	196	LEU
1	A	212	GLN
1	A	217	ILE
1	A	222	ASN
1	A	230	LEU
1	A	254	GLU
1	A	272	CYS
1	A	280	GLN
1	A	309	SER
1	A	323	LYS
1	A	337	LYS
1	A	340	VAL
1	A	401	LYS
1	B	14	GLU
1	B	20	GLU
1	B	21	VAL
1	B	46	LEU
1	B	57	GLU
1	B	58	ARG
1	B	78	LEU
1	B	80	ARG
1	B	99	VAL
1	B	107	ILE
1	B	116	LYS
1	B	125	VAL
1	B	168	LEU
1	B	180	VAL
1	B	186	LYS
1	B	190	MET
1	B	191	GLN
1	B	196	LEU

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Mol	Chain	Res	Type
1	B	212	GLN
1	B	217	ILE
1	B	222	ASN
1	B	230	LEU
1	B	248	VAL
1	B	254	GLU
1	B	272	CYS
1	B	337	LYS
1	B	340	VAL
1	B	392	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	69	HIS
1	A	220	HIS
1	A	242	GLN
1	A	293	GLN
1	B	16	HIS
1	B	37	ASN
1	B	45	HIS
1	B	63	ASN
1	B	191	GLN
1	B	212	GLN
1	B	218	HIS
1	B	220	HIS
1	B	242	GLN
1	B	287	HIS
1	B	293	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
3	PIM	B	1501	2	11,12,12	2.44	5 (45%)	14,15,15	3.14	8 (57%)
4	NHE	B	1502	-	13,13,13	2.45	3 (23%)	16,17,17	1.01	1 (6%)
3	PIM	A	501	2	11,12,12	2.60	4 (36%)	14,15,15	3.12	7 (50%)
4	NHE	B	1503	-	13,13,13	2.29	3 (23%)	16,17,17	1.05	1 (6%)
4	NHE	A	503	-	13,13,13	3.32	4 (30%)	16,17,17	1.36	3 (18%)
4	NHE	A	502	-	13,13,13	3.24	1 (7%)	16,17,17	0.91	1 (6%)
2	HEM	A	404	1,3	50,50,50	1.64	9 (18%)	67,82,82	1.29	9 (13%)
2	HEM	B	404	1,3	50,50,50	1.77	13 (26%)	67,82,82	1.29	8 (11%)

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	PIM	B	1501	2	-	0/4/4/4	0/2/2/2
4	NHE	B	1502	-	-	2/7/15/15	0/1/1/1
3	PIM	A	501	2	-	0/4/4/4	0/2/2/2
4	NHE	B	1503	-	-	2/7/15/15	0/1/1/1
4	NHE	A	503	-	-	1/7/15/15	0/1/1/1
4	NHE	A	502	-	-	2/7/15/15	0/1/1/1
2	HEM	A	404	1,3	-	7/14/54/54	-
2	HEM	B	404	1,3	-	9/14/54/54	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	NHE	C2-S	-11.37	1.61	1.77
4	A	503	NHE	C1-N	9.51	1.67	1.47
4	B	1502	NHE	C2-S	-7.57	1.67	1.77
4	B	1503	NHE	C2-S	-7.02	1.67	1.77
2	A	404	HEM	FE-NC	5.75	2.14	1.95
3	A	501	PIM	C4-N3	-5.75	1.27	1.37
2	B	404	HEM	FE-NC	5.54	2.13	1.95
4	A	503	NHE	C2'-C1'	5.32	1.64	1.52
3	B	1501	PIM	C4-N3	-5.06	1.28	1.37
3	A	501	PIM	C8-C7	3.87	1.45	1.38
3	B	1501	PIM	C8-C7	3.86	1.45	1.38
4	A	503	NHE	C2-S	-3.59	1.72	1.77
2	B	404	HEM	FE-NA	3.38	2.06	1.95
3	A	501	PIM	C6-C5	3.16	1.52	1.47
2	B	404	HEM	C4A-NA	-3.08	1.33	1.39
2	B	404	HEM	CHD-C4C	3.02	1.44	1.38
2	A	404	HEM	CMB-C2B	2.76	1.56	1.50
2	A	404	HEM	C4A-NA	-2.70	1.34	1.39
4	B	1503	NHE	C2'-C1'	2.66	1.58	1.52
2	B	404	HEM	FE-ND	2.61	2.02	1.94
2	B	404	HEM	CMB-C2B	2.52	1.55	1.50
2	B	404	HEM	C1C-NC	-2.45	1.35	1.39
3	A	501	PIM	C5-N1	-2.45	1.35	1.38
2	B	404	HEM	CHD-C1D	2.43	1.44	1.39
2	B	404	HEM	CBB-CAB	2.43	1.42	1.30
2	A	404	HEM	CBB-CAB	2.43	1.42	1.30
4	B	1502	NHE	O1-S	-2.42	1.38	1.45
2	B	404	HEM	CAC-C3C	-2.36	1.41	1.47
2	A	404	HEM	C1A-NA	-2.28	1.35	1.39
2	A	404	HEM	O1A-CGA	2.28	1.29	1.22
3	B	1501	PIM	C5-N1	-2.27	1.35	1.38
2	B	404	HEM	CBD-CGD	2.25	1.55	1.50
2	B	404	HEM	C1A-NA	-2.18	1.35	1.39
2	A	404	HEM	FE-NA	2.14	2.02	1.95
4	B	1503	NHE	C6'-C1'	2.13	1.56	1.52
2	B	404	HEM	CAD-C3D	2.12	1.56	1.51
4	A	503	NHE	O3-S	-2.12	1.39	1.47
3	B	1501	PIM	C10-C11	2.09	1.42	1.38
2	A	404	HEM	CAC-C3C	-2.08	1.41	1.47
4	B	1502	NHE	O2-S	2.08	1.51	1.45
3	B	1501	PIM	C6-C5	2.07	1.50	1.47
2	A	404	HEM	CMC-C2C	2.05	1.55	1.50

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	PIM	C2-N1-C5	-7.97	103.46	107.53
3	B	1501	PIM	C2-N1-C5	-7.94	103.48	107.53
3	B	1501	PIM	C10-C9-C8	4.28	125.73	119.87
3	A	501	PIM	C10-C9-C8	4.13	125.53	119.87
2	B	404	HEM	CBA-CAA-C2A	3.69	122.74	112.53
3	B	1501	PIM	C11-C6-C7	3.58	123.12	118.57
2	A	404	HEM	CBA-CAA-C2A	3.58	122.43	112.53
3	A	501	PIM	C11-C6-C7	3.56	123.09	118.57
2	B	404	HEM	CBD-CAD-C3D	3.52	122.26	112.53
2	A	404	HEM	CBD-CAD-C3D	3.39	121.92	112.53
2	A	404	HEM	CAD-CBD-CGD	3.36	122.58	113.67
3	B	1501	PIM	C9-C10-C11	-3.23	116.26	120.24
2	A	404	HEM	C4B-C3B-C2B	-3.17	104.37	107.28
3	A	501	PIM	C9-C10-C11	-3.16	116.34	120.24
2	B	404	HEM	CAD-CBD-CGD	3.06	121.79	113.67
4	A	503	NHE	O3-S-O2	2.92	118.70	111.40
2	B	404	HEM	C4B-C3B-C2B	-2.92	104.60	107.28
4	A	503	NHE	C1-N-C1'	2.88	119.73	114.18
3	B	1501	PIM	C9-C8-C7	-2.83	116.75	120.24
4	B	1503	NHE	O1-S-C2	-2.83	102.46	106.73
3	A	501	PIM	C9-C8-C7	-2.78	116.81	120.24
2	A	404	HEM	CAA-CBA-CGA	2.76	120.97	113.67
2	B	404	HEM	CAA-CBA-CGA	2.66	120.71	113.67
2	B	404	HEM	C3B-C4B-NB	2.58	111.32	109.47
3	A	501	PIM	C6-C5-N1	2.57	126.70	123.72
2	B	404	HEM	O2D-CGD-CBD	2.50	121.89	114.00
4	B	1502	NHE	O1-S-C2	-2.49	102.96	106.73
4	A	503	NHE	O2-S-C2	-2.49	102.97	106.73
4	A	502	NHE	C2-C1-N	-2.48	104.34	111.40
3	B	1501	PIM	C6-C5-N1	2.43	126.54	123.72
2	A	404	HEM	O2D-CGD-CBD	2.39	121.56	114.00
2	B	404	HEM	O1D-CGD-CBD	-2.33	115.71	123.09
3	B	1501	PIM	C8-C7-C6	-2.32	118.09	120.36
3	A	501	PIM	C8-C7-C6	-2.30	118.10	120.36
2	A	404	HEM	O1D-CGD-CBD	-2.26	115.94	123.09
2	A	404	HEM	C3B-C4B-NB	2.21	111.06	109.47
3	B	1501	PIM	C7-C6-C5	-2.09	117.63	120.81
2	A	404	HEM	C4C-C3C-C2C	-2.02	105.06	106.81

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	404	HEM	C2C-C3C-CAC-CBC
2	A	404	HEM	C4C-C3C-CAC-CBC
2	B	404	HEM	C2C-C3C-CAC-CBC
2	B	404	HEM	C4C-C3C-CAC-CBC
4	A	502	NHE	C2'-C1'-N-C1
4	A	503	NHE	C2-C1-N-C1'
4	B	1502	NHE	C2'-C1'-N-C1
2	B	404	HEM	C2A-CAA-CBA-CGA
4	B	1502	NHE	C2-C1-N-C1'
2	A	404	HEM	C2A-CAA-CBA-CGA
4	B	1503	NHE	C2-C1-N-C1'
2	B	404	HEM	CAA-CBA-CGA-O2A
2	A	404	HEM	CAD-CBD-CGD-O1D
2	A	404	HEM	CAA-CBA-CGA-O2A
2	B	404	HEM	CAA-CBA-CGA-O1A
2	B	404	HEM	CAD-CBD-CGD-O2D
2	A	404	HEM	CAA-CBA-CGA-O1A
2	B	404	HEM	CAD-CBD-CGD-O1D
4	A	502	NHE	C6'-C1'-N-C1
2	A	404	HEM	CAD-CBD-CGD-O2D
2	B	404	HEM	C4B-C3B-CAB-CBB
4	B	1503	NHE	C6'-C1'-N-C1
2	B	404	HEM	C2B-C3B-CAB-CBB

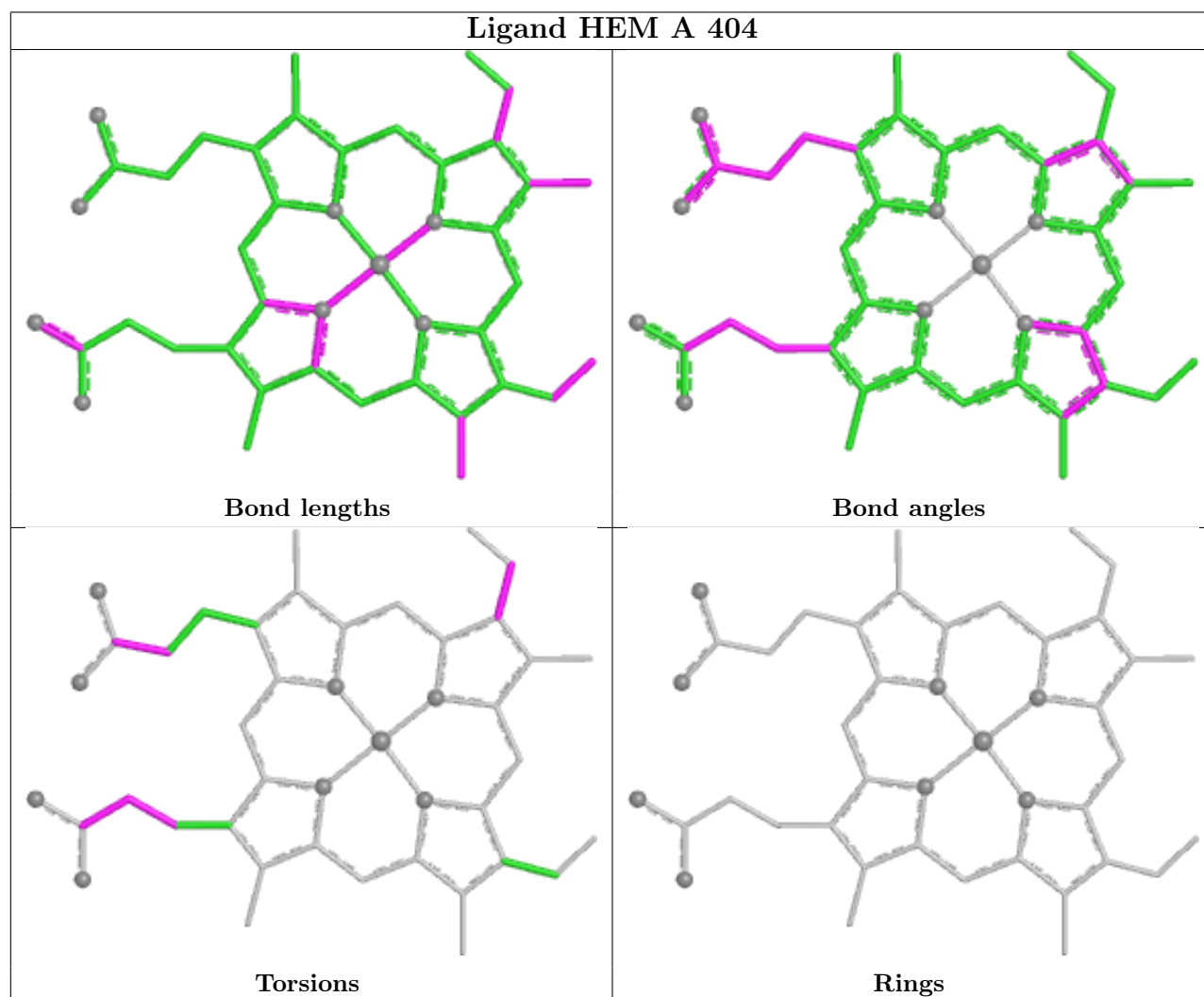
There are no ring outliers.

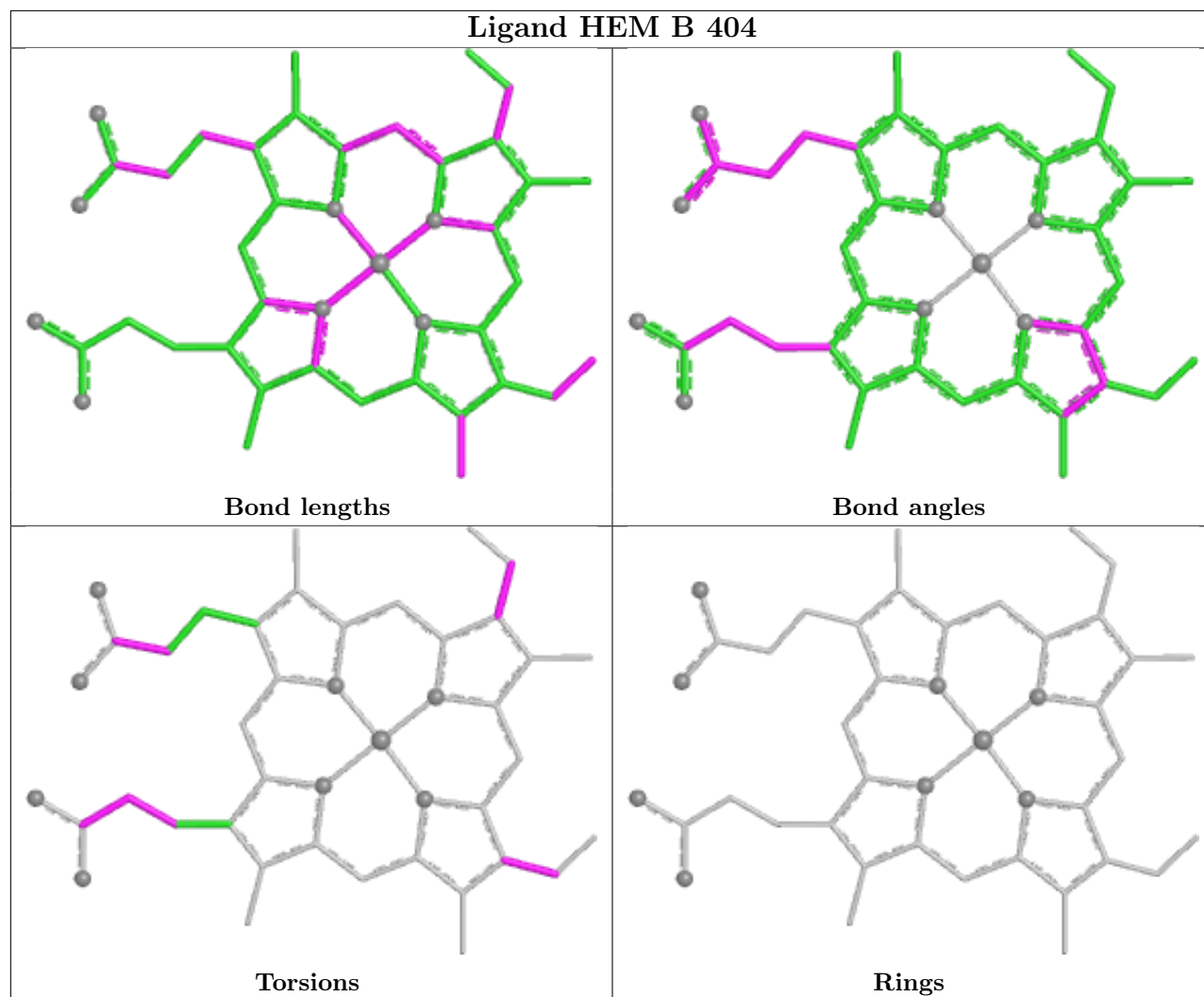
8 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1501	PIM	2	0
4	B	1502	NHE	2	0
3	A	501	PIM	2	0
4	B	1503	NHE	3	0
4	A	503	NHE	7	0
4	A	502	NHE	2	0
2	A	404	HEM	6	0
2	B	404	HEM	5	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	373/406 (91%)	-0.33	3 (0%) 82 83	36, 54, 82, 127	0
1	B	374/406 (92%)	-0.23	8 (2%) 63 65	35, 55, 85, 109	0
All	All	747/812 (91%)	-0.28	11 (1%) 72 73	35, 54, 84, 127	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	11	ILE	5.1
1	B	380	GLY	3.4
1	A	381	GLY	3.3
1	B	381	GLY	3.2
1	B	402	GLU	2.9
1	A	403	GLY	2.6
1	B	396	GLU	2.5
1	B	403	GLY	2.5
1	B	308	CYS	2.5
1	A	401	LYS	2.5
1	B	382	THR	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

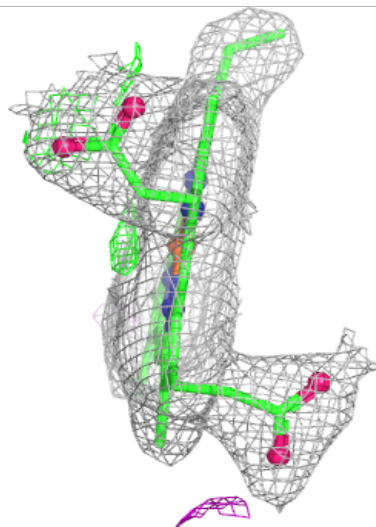
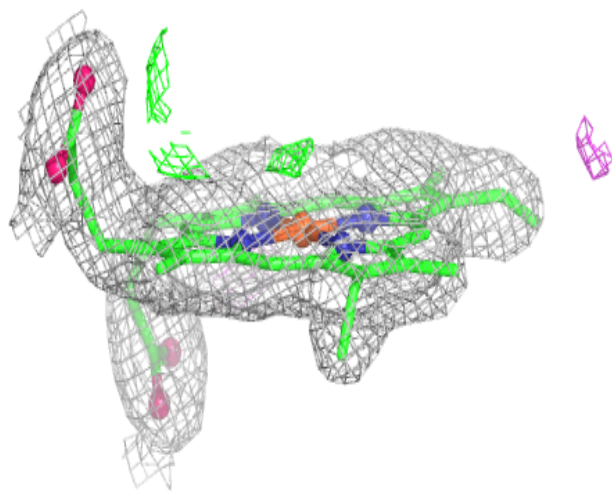
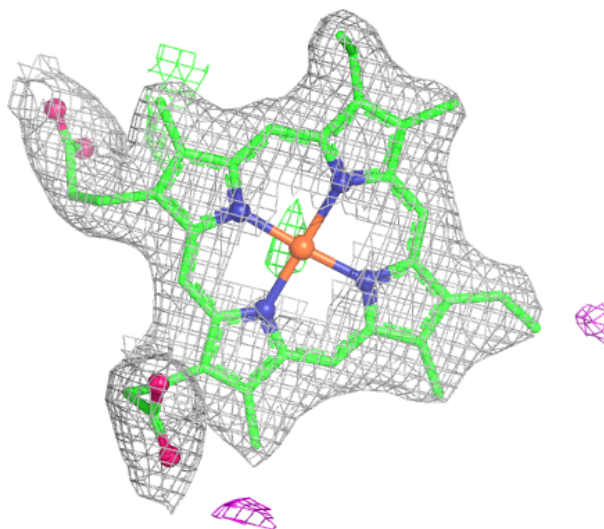
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	NHE	A	503	13/13	0.74	0.21	70,88,127,128	0
4	NHE	A	502	13/13	0.81	0.20	66,83,109,111	0
4	NHE	B	1502	13/13	0.85	0.17	66,76,110,116	0
4	NHE	B	1503	13/13	0.86	0.14	66,72,110,111	0
3	PIM	A	501	11/11	0.98	0.05	28,34,39,40	0
3	PIM	B	1501	11/11	0.98	0.04	35,40,45,47	0
2	HEM	A	404	43/43	0.99	0.06	28,41,48,55	0
2	HEM	B	404	43/43	0.99	0.07	33,42,55,60	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.

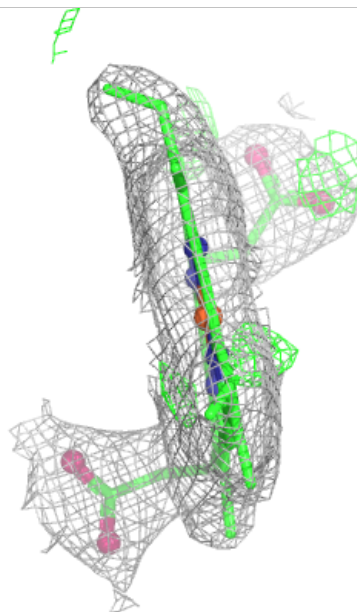
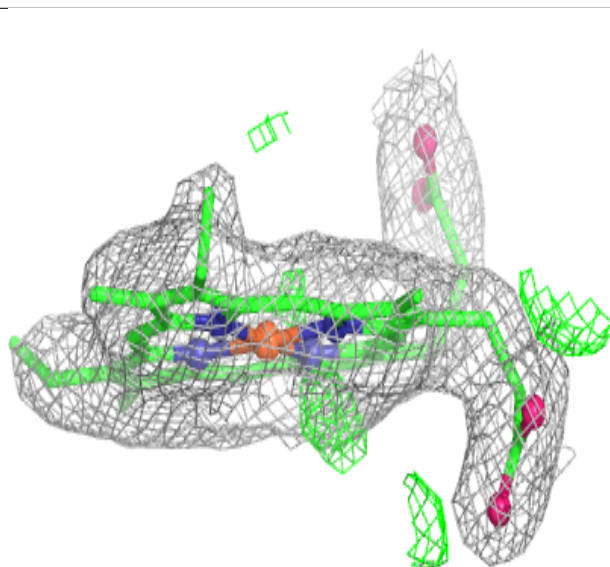
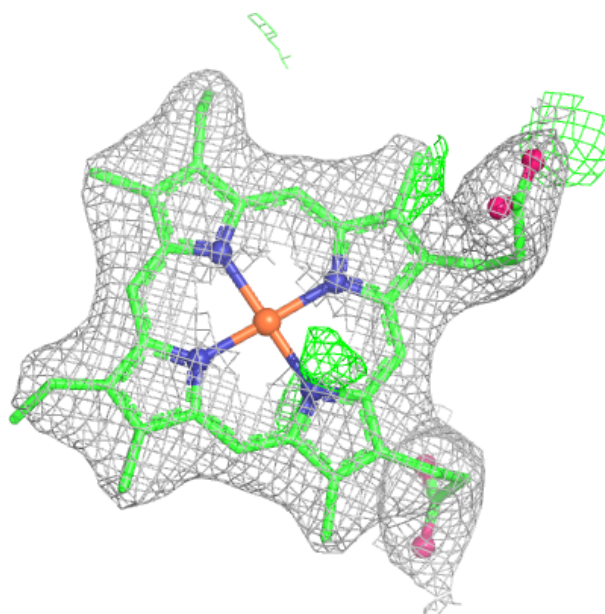
Electron density around HEM A 404:

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



Electron density around HEM B 404:

$2mF_o-DF_c$ (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.