



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 06:24 pm BST

PDB ID : 2D0U  
Title : Crystal structure of cyanide 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 : 3.40 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

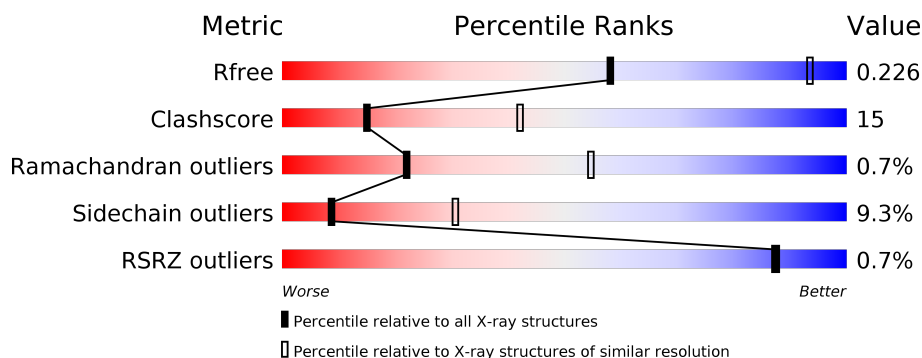
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0;">%</div> <div style="position: absolute; top: 0; left: 0; width: 63%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 63%; width: 25%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 88%; width: 8%; height: 10px; background-color: red;"></div> <div style="position: absolute; top: 0; left: 88%; width: 8%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>63%</span> <span>25%</span> <span>• • 8%</span> </div> </div>
1	B	406	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 0; left: 0; width: 64%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 64%; width: 24%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 88%; width: 8%; height: 10px; background-color: red;"></div> <div style="position: absolute; top: 0; left: 88%; width: 8%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>64%</span> <span>24%</span> <span>• 8%</span> </div> </div>

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
2	CYN	A	405	-	-	X	-
2	CYN	B	1405	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6062 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.

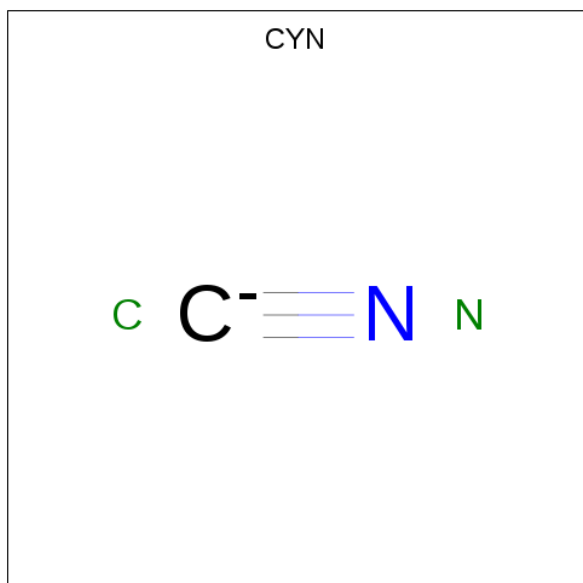
- Molecule 1 is a protein called Indoleamine 2,3-dioxygenase.

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	374	Total	C	N	O	S	0	0	0
			2964	1905	505	537	17			

There are 6 discrepancies between the modelled and reference sequences:

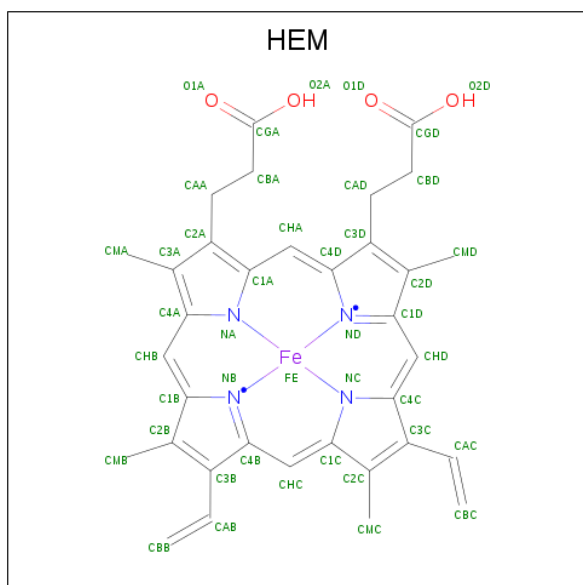
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	CLONING ARTIFACT	UNP P14902
A	-1	SER	-	CLONING ARTIFACT	UNP P14902
A	0	HIS	-	CLONING ARTIFACT	UNP P14902
B	-2	GLY	-	CLONING ARTIFACT	UNP P14902
B	-1	SER	-	CLONING ARTIFACT	UNP P14902
B	0	HIS	-	CLONING ARTIFACT	UNP P14902

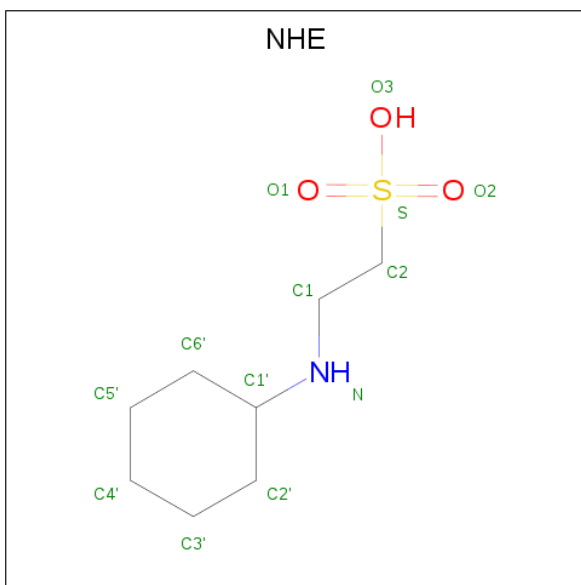
- Molecule 2 is CYANIDE ION (three-letter code: CYN) (formula: CN).



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

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



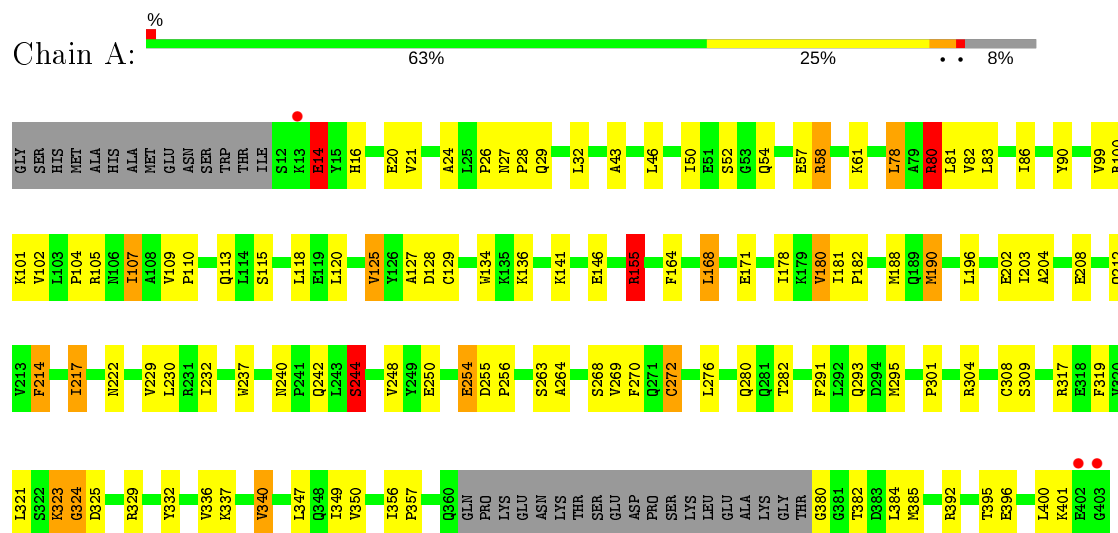


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
4	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
4	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
4	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

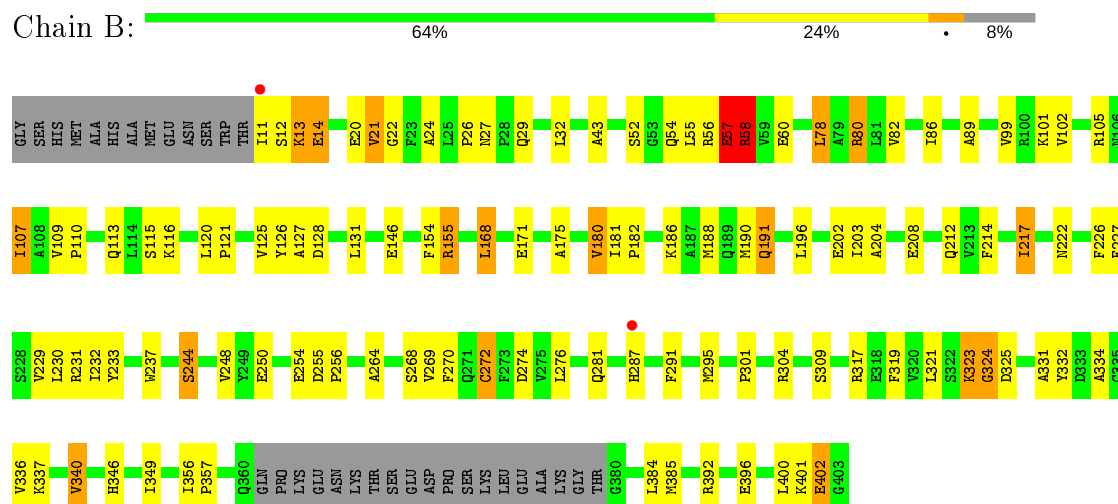
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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



- Molecule 1: Indoleamine 2,3-dioxygenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.35Å 97.09Å 129.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.73 – 3.40 19.73 – 3.40	Depositor EDS
% Data completeness (in resolution range)	93.5 (19.73-3.40) 93.6 (19.73-3.40)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.55 (at 3.44Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.213 , 0.254 0.191 , 0.226	Depositor DCC
$R_{free}$ test set	718 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.2	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 37.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6062	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NHE, HEM, CYN

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	0.61	8/3024 (0.3%)	0.69	1/4087 (0.0%)
1	B	0.60	8/3032 (0.3%)	0.71	4/4098 (0.1%)
All	All	0.60	16/6056 (0.3%)	0.70	5/8185 (0.1%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	323	LYS	C-O	-8.59	1.07	1.23
1	B	323	LYS	C-O	-8.33	1.07	1.23
1	B	146	GLU	CD-OE1	-7.33	1.17	1.25
1	A	202	GLU	CD-OE1	-7.13	1.17	1.25
1	B	202	GLU	CD-OE1	-7.08	1.17	1.25
1	A	146	GLU	CD-OE1	-6.90	1.18	1.25
1	A	80	ARG	CZ-NH1	-6.64	1.24	1.33
1	B	80	ARG	CZ-NH1	-6.40	1.24	1.33
1	B	244	SER	CB-OG	-6.36	1.33	1.42
1	A	244	SER	CB-OG	-5.65	1.34	1.42
1	A	57	GLU	CD-OE1	-5.55	1.19	1.25
1	B	155	ARG	CZ-NH1	-5.39	1.26	1.33
1	B	57	GLU	CD-OE1	-5.38	1.19	1.25
1	A	155	ARG	CZ-NH1	-5.15	1.26	1.33
1	A	396	GLU	CB-CG	-5.11	1.42	1.52
1	B	58	ARG	CG-CD	-5.01	1.39	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	58	ARG	NE-CZ-NH1	-9.30	115.65	120.30
1	A	80	ARG	NE-CZ-NH2	6.03	123.31	120.30
1	B	80	ARG	NE-CZ-NH2	5.82	123.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	155	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	B	155	ARG	NE-CZ-NH1	-5.16	117.72	120.30

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	98	1
1	B	2964	0	2978	82	1
2	A	2	0	0	2	0
2	B	2	0	0	2	0
3	A	43	0	30	4	0
3	B	43	0	30	4	0
4	A	26	0	32	6	0
4	B	26	0	32	4	0
All	All	6062	0	6069	183	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 15.

All (183) 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:402:GLU:O	1:B:402:GLU:HG3	1.46	1.11
1:B:323:LYS:O	1:B:325:ASP:N	2.00	0.95
1:B:401:LYS:HG2	1:B:402:GLU:H	1.31	0.94
1:B:21:VAL:HG13	1:B:24:ALA:HB3	1.50	0.90
1:A:401:LYS:HA	1:A:401:LYS:HE2	1.55	0.88
1:B:401:LYS:HG2	1:B:402:GLU:N	1.87	0.88
1:B:401:LYS:CG	1:B:402:GLU:H	1.89	0.86
1:A:323:LYS:O	1:A:325:ASP:N	2.09	0.84
1:A:58:ARG:HH11	1:A:58:ARG:HG3	1.43	0.83
1:B:80:ARG:NH2	1:B:121:PRO:O	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:VAL:HG13	1:A:24:ALA:HB3	1.57	0.83
2:A:405:CYN:N	4:A:406:NHE:H5'2	1.93	0.82
1:B:105:ARG:HB3	1:B:250:GLU:HG2	1.62	0.81
1:A:217:ILE:HG21	1:A:349:ILE:HD13	1.62	0.81
1:A:188:MET:HG2	1:A:319:PHE:CD2	2.17	0.80
1:B:13:LYS:HD2	1:B:14:GLU:H	1.47	0.76
1:A:263:SER:CB	4:A:406:NHE:H6'1	2.15	0.75
1:A:264:ALA:HB3	2:A:405:CYN:C	2.17	0.74
1:B:226:PHE:HZ	4:B:1406:NHE:H4'2	1.52	0.74
1:B:102:VAL:HG22	1:B:248:VAL:HG11	1.71	0.73
1:A:136:LYS:HE2	1:A:141:LYS:O	1.88	0.72
1:B:21:VAL:CG1	1:B:24:ALA:HB3	2.22	0.68
1:A:28:PRO:HG2	1:A:134:TRP:O	1.93	0.67
1:B:287:HIS:CE1	4:B:1407:NHE:H4'2	2.28	0.67
1:B:356:ILE:HB	1:B:357:PRO:HD3	1.76	0.67
1:B:255:ASP:HB3	1:B:256:PRO:HD2	1.76	0.67
1:A:329:ARG:HE	1:A:401:LYS:HD2	1.60	0.66
1:B:402:GLU:O	1:B:402:GLU:CG	2.30	0.66
1:A:102:VAL:HG22	1:A:248:VAL:HG11	1.76	0.66
1:B:102:VAL:HG22	1:B:248:VAL:CG1	2.26	0.66
1:B:52:SER:OG	1:B:54:GLN:HG3	1.97	0.65
1:A:217:ILE:HG21	1:A:349:ILE:CD1	2.26	0.65
1:A:102:VAL:HG22	1:A:248:VAL:CG1	2.27	0.65
1:A:323:LYS:O	1:A:324:GLY:C	2.32	0.65
1:A:217:ILE:HD13	1:A:217:ILE:O	1.97	0.64
1:A:356:ILE:HB	1:A:357:PRO:HD3	1.79	0.63
1:B:24:ALA:HA	1:B:131:LEU:HD22	1.81	0.62
1:A:52:SER:OG	1:A:54:GLN:HG2	2.00	0.62
1:A:27:ASN:O	1:A:27:ASN:ND2	2.33	0.61
1:A:263:SER:HB2	4:A:406:NHE:H6'1	1.82	0.61
1:B:323:LYS:O	1:B:324:GLY:C	2.38	0.61
1:B:321:LEU:HD21	1:B:400:LEU:HD22	1.82	0.60
1:B:13:LYS:CD	1:B:14:GLU:H	2.15	0.59
1:B:301:PRO:HA	1:B:304:ARG:NH1	2.17	0.59
1:A:329:ARG:NE	1:A:401:LYS:HD2	2.17	0.59
1:A:301:PRO:HA	1:A:304:ARG:NH1	2.17	0.59
1:A:255:ASP:HB3	1:A:256:PRO:HD2	1.85	0.59
1:B:102:VAL:HA	1:B:248:VAL:HG13	1.85	0.58
1:B:56:ARG:O	1:B:60:GLU:HG3	2.03	0.58
1:A:14:GLU:C	1:A:16:HIS:H	2.06	0.58
1:A:321:LEU:HD21	1:A:400:LEU:HD22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ALA:HB2	1:B:82:VAL:HG13	1.86	0.58
1:A:347:LEU:HD12	1:A:392:ARG:HH11	1.68	0.57
1:B:217:ILE:HG21	1:B:349:ILE:HD12	1.87	0.57
1:B:171:GLU:OE2	1:B:269:VAL:HG23	2.05	0.57
1:B:32:LEU:HG	1:B:78:LEU:HD13	1.85	0.57
1:A:58:ARG:CG	1:A:58:ARG:HH11	2.15	0.56
1:B:180:VAL:HG21	1:B:203:ILE:HG13	1.86	0.56
1:A:204:ALA:O	1:A:208:GLU:HG3	2.05	0.55
1:A:21:VAL:CG1	1:A:24:ALA:HB3	2.34	0.55
1:B:384:LEU:HD21	3:B:404:HEM:HMA3	1.88	0.55
1:A:181:ILE:HD12	1:A:276:LEU:HG	1.87	0.55
1:B:11:ILE:HG22	1:B:12:SER:N	2.22	0.54
1:A:21:VAL:O	1:A:21:VAL:HG13	2.05	0.54
1:A:188:MET:HG2	1:A:319:PHE:CE2	2.41	0.54
1:B:57:GLU:HG3	1:B:58:ARG:N	2.16	0.54
1:B:107:ILE:O	1:B:110:PRO:HD2	2.08	0.54
1:A:190:MET:HA	1:A:190:MET:CE	2.38	0.53
1:A:58:ARG:CG	1:A:58:ARG:NH1	2.70	0.53
1:A:171:GLU:OE2	1:A:269:VAL:HG23	2.09	0.53
1:A:317:ARG:HD2	1:A:332:TYR:OH	2.08	0.53
4:A:406:NHE:HC21	4:A:407:NHE:HN	1.73	0.53
1:B:317:ARG:HD2	1:B:332:TYR:OH	2.08	0.53
1:A:269:VAL:HG12	1:A:270:PHE:CD1	2.43	0.53
1:B:287:HIS:HE1	4:B:1407:NHE:H4'2	1.71	0.53
1:B:384:LEU:HD11	3:B:404:HEM:HMA3	1.91	0.53
1:A:181:ILE:HB	1:A:182:PRO:HD3	1.91	0.53
1:A:80:ARG:HG3	1:A:118:LEU:HD12	1.90	0.53
1:A:180:VAL:HG21	1:A:203:ILE:HG13	1.90	0.52
1:A:263:SER:HA	4:A:406:NHE:H6'1	1.90	0.52
1:A:263:SER:CA	4:A:406:NHE:H6'1	2.39	0.52
1:A:101:LYS:O	1:A:248:VAL:HG12	2.10	0.52
1:B:155:ARG:HD2	1:B:233:TYR:OH	2.10	0.52
1:A:268:SER:O	1:A:272:CYS:HB3	2.10	0.52
1:A:295:MET:HE2	1:A:295:MET:HA	1.91	0.51
1:B:101:LYS:O	1:B:248:VAL:HG12	2.09	0.51
1:B:188:MET:HG2	1:B:319:PHE:CD2	2.46	0.51
1:B:109:VAL:O	1:B:113:GLN:HG3	2.10	0.51
1:B:127:ALA:HA	1:B:131:LEU:HD12	1.93	0.51
1:B:82:VAL:O	1:B:86:ILE:HG13	2.11	0.50
1:A:32:LEU:HG	1:A:78:LEU:HD13	1.92	0.50
1:A:384:LEU:HD11	3:A:404:HEM:HMA3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:VAL:HB	1:A:110:PRO:HD3	1.94	0.50
1:B:168:LEU:O	1:B:171:GLU:HB3	2.12	0.50
1:B:385:MET:HA	1:B:385:MET:HE2	1.94	0.50
1:A:269:VAL:HG12	1:A:270:PHE:HD1	1.77	0.50
1:A:58:ARG:HG3	1:A:58:ARG:NH1	2.17	0.50
1:B:181:ILE:HB	1:B:182:PRO:HD3	1.94	0.50
1:B:29:GLN:O	1:B:78:LEU:HG	2.12	0.49
1:A:105:ARG:HB3	1:A:250:GLU:HG2	1.93	0.49
1:A:350:VAL:HG11	1:A:385:MET:CE	2.43	0.49
1:A:384:LEU:HD11	3:A:404:HEM:CMA	2.42	0.49
1:A:254:GLU:H	1:A:254:GLU:CD	2.15	0.49
1:A:282:THR:CG2	1:A:293:GLN:OE1	2.60	0.49
1:B:268:SER:O	1:B:272:CYS:HB3	2.13	0.48
1:B:270:PHE:CD1	1:B:270:PHE:N	2.81	0.48
1:A:115:SER:HB3	1:A:120:LEU:O	2.14	0.48
1:A:29:GLN:O	1:A:78:LEU:HG	2.14	0.48
1:A:43:ALA:HB2	1:A:82:VAL:HG13	1.96	0.48
1:B:191:GLN:CA	1:B:191:GLN:HE21	2.26	0.48
1:B:154:PHE:O	1:B:155:ARG:HG2	2.14	0.47
1:B:336:VAL:O	1:B:340:VAL:HG13	2.14	0.47
1:B:109:VAL:HB	1:B:110:PRO:HD3	1.96	0.47
1:B:21:VAL:O	1:B:21:VAL:HG13	2.14	0.47
1:A:384:LEU:HD21	3:A:404:HEM:HMA3	1.95	0.47
1:A:107:ILE:O	1:A:110:PRO:HD2	2.13	0.47
1:B:269:VAL:HG12	1:B:270:PHE:CD1	2.49	0.47
1:A:214:PHE:CE1	1:A:349:ILE:HD12	2.49	0.47
1:A:21:VAL:O	1:A:21:VAL:CG1	2.63	0.47
1:B:14:GLU:CD	1:B:14:GLU:N	2.68	0.47
1:B:384:LEU:HD11	3:B:404:HEM:CMA	2.45	0.47
1:A:282:THR:HG21	1:A:293:GLN:OE1	2.15	0.47
1:A:401:LYS:HE2	1:A:401:LYS:CA	2.37	0.47
1:A:102:VAL:HA	1:A:248:VAL:HG13	1.96	0.46
1:A:80:ARG:NH2	1:A:128:ASP:OD2	2.46	0.46
1:A:269:VAL:HG12	1:A:270:PHE:N	2.30	0.46
1:B:21:VAL:CG1	1:B:21:VAL:O	2.63	0.46
1:B:115:SER:HB3	1:B:120:LEU:O	2.15	0.46
1:A:83:LEU:HD22	1:A:107:ILE:HD11	1.98	0.46
1:B:269:VAL:HG12	1:B:270:PHE:N	2.31	0.45
1:A:50:ILE:HG21	1:A:155:ARG:HE	1.78	0.45
1:A:155:ARG:HB3	1:A:155:ARG:HH11	1.81	0.45
1:A:100:ARG:HA	1:A:100:ARG:HD3	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ALA:O	1:B:208:GLU:HG3	2.16	0.45
1:B:264:ALA:HB3	2:B:1405:CYN:C	2.47	0.45
1:B:191:GLN:HA	1:B:191:GLN:HE21	1.82	0.45
1:A:282:THR:HG22	1:A:282:THR:O	2.16	0.45
1:B:274:ASP:OD2	1:B:281:GLN:HG3	2.17	0.45
3:B:404:HEM:HBA1	4:B:1407:NHE:H6'2	1.99	0.45
1:A:319:PHE:CE1	1:A:323:LYS:HE2	2.52	0.44
1:B:13:LYS:NZ	1:B:14:GLU:HB2	2.32	0.44
1:B:80:ARG:NH1	1:B:128:ASP:OD2	2.51	0.44
1:A:350:VAL:HG11	1:A:385:MET:HE1	1.99	0.44
1:A:78:LEU:O	1:A:81:LEU:HB3	2.18	0.44
1:A:270:PHE:N	1:A:270:PHE:CD1	2.86	0.43
1:A:282:THR:CG2	1:A:282:THR:O	2.66	0.43
1:B:264:ALA:HB3	2:B:1405:CYN:N	2.34	0.43
1:A:336:VAL:O	1:A:340:VAL:HG13	2.18	0.43
1:A:125:VAL:HG13	1:A:127:ALA:H	1.83	0.43
1:B:217:ILE:HD13	1:B:217:ILE:O	2.17	0.43
1:A:385:MET:HA	1:A:385:MET:HE2	2.00	0.43
1:B:291:PHE:O	1:B:295:MET:HG2	2.18	0.43
1:A:178:ILE:O	1:A:181:ILE:HG12	2.19	0.43
1:B:27:ASN:O	1:B:27:ASN:ND2	2.52	0.43
1:A:90:TYR:CE2	1:A:104:PRO:HD3	2.53	0.42
1:A:181:ILE:CD1	1:A:276:LEU:HG	2.49	0.42
1:B:126:TYR:CD1	1:B:264:ALA:HA	2.54	0.42
1:A:14:GLU:C	1:A:14:GLU:CD	2.78	0.42
1:B:346:HIS:O	1:B:349:ILE:HB	2.18	0.42
1:B:331:ALA:O	1:B:334:ALA:HB3	2.20	0.42
1:B:229:VAL:O	1:B:232:ILE:HB	2.20	0.42
1:B:55:LEU:HD22	1:B:89:ALA:HB1	2.01	0.42
1:A:82:VAL:O	1:A:86:ILE:HG13	2.19	0.41
1:B:319:PHE:CD1	1:B:319:PHE:C	2.94	0.41
1:A:109:VAL:O	1:A:113:GLN:HG3	2.20	0.41
1:A:340:VAL:HG12	1:A:395:THR:HG22	2.02	0.41
1:A:270:PHE:HD1	1:A:270:PHE:N	2.19	0.41
1:A:380:GLY:C	1:A:382:THR:H	2.23	0.41
1:B:22:GLY:HA3	1:B:175:ALA:CB	2.50	0.41
1:B:26:PRO:O	1:B:27:ASN:C	2.58	0.41
1:A:136:LYS:CE	1:A:141:LYS:O	2.65	0.41
1:B:270:PHE:H	1:B:270:PHE:HD1	1.69	0.41
1:A:240:ASN:OD1	1:A:242:GLN:HG2	2.20	0.41
1:B:227:PHE:O	1:B:231:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LEU:O	1:A:171:GLU:HB3	2.20	0.40
1:B:13:LYS:CD	1:B:14:GLU:N	2.83	0.40
1:A:129:CYS:HB2	1:A:164:PHE:CZ	2.56	0.40
1:A:26:PRO:O	1:A:27:ASN:C	2.59	0.40
1:B:181:ILE:CD1	1:B:276:LEU:HG	2.51	0.40
1:A:14:GLU:C	1:A:16:HIS:N	2.73	0.40
1:A:384:LEU:HD11	3:A:404:HEM:HAA1	2.03	0.40
1:A:291:PHE:O	1:A:295:MET:HG2	2.21	0.40
1:A:229:VAL:O	1:A:232:ILE:HB	2.22	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:100:ARG:NH2	1:B:402:GLU:OE1[3_655]	2.08	0.12

## 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	369/406 (91%)	346 (94%)	20 (5%)	3 (1%)	19	51
1	B	370/406 (91%)	349 (94%)	19 (5%)	2 (0%)	29	61
All	All	739/812 (91%)	695 (94%)	39 (5%)	5 (1%)	22	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	GLY
1	B	324	GLY
1	B	244	SER
1	A	244	SER

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Mol	Chain	Res	Type
1	A	14	GLU

### 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%)	293 (91%)	29 (9%)	9	32
1	B	323/350 (92%)	292 (90%)	31 (10%)	8	29
All	All	645/700 (92%)	585 (91%)	60 (9%)	9	31

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	20	GLU
1	A	46	LEU
1	A	58	ARG
1	A	61	LYS
1	A	78	LEU
1	A	80	ARG
1	A	99	VAL
1	A	107	ILE
1	A	125	VAL
1	A	155	ARG
1	A	168	LEU
1	A	180	VAL
1	A	190	MET
1	A	196	LEU
1	A	212	GLN
1	A	214	PHE
1	A	217	ILE
1	A	222	ASN
1	A	230	LEU
1	A	237	TRP
1	A	244	SER

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Mol	Chain	Res	Type
1	A	254	GLU
1	A	272	CYS
1	A	280	GLN
1	A	308	CYS
1	A	309	SER
1	A	337	LYS
1	A	340	VAL
1	B	13	LYS
1	B	14	GLU
1	B	20	GLU
1	B	21	VAL
1	B	57	GLU
1	B	58	ARG
1	B	78	LEU
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
1	B	212	GLN
1	B	214	PHE
1	B	217	ILE
1	B	222	ASN
1	B	230	LEU
1	B	237	TRP
1	B	254	GLU
1	B	272	CYS
1	B	309	SER
1	B	337	LYS
1	B	340	VAL
1	B	392	ARG
1	B	396	GLU
1	B	402	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	37	ASN
1	A	69	HIS
1	A	212	GLN
1	A	242	GLN
1	B	37	ASN
1	B	63	ASN
1	B	191	GLN
1	B	212	GLN
1	B	287	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	CYN	B	1405	3	0,1,1	0.00	-	-		
4	NHE	B	1407	-	13,13,13	1.43	2 (15%)	16,17,17	1.05	1 (6%)
3	HEM	B	404	1,2	27,50,50	1.55	4 (14%)	17,82,82	3.64	6 (35%)
3	HEM	A	404	1,2	27,50,50	1.34	3 (11%)	17,82,82	3.40	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NHE	A	406	-	13,13,13	1.68	1 (7%)	16,17,17	1.12	1 (6%)
4	NHE	B	1406	-	13,13,13	1.53	1 (7%)	16,17,17	1.05	1 (6%)
4	NHE	A	407	-	13,13,13	1.54	2 (15%)	16,17,17	0.82	0
2	CYN	A	405	3	0,1,1	0.00	-	-		

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
4	NHE	B	1407	-	-	2/7/15/15	0/1/1/1
3	HEM	B	404	1,2	-	1/6/54/54	-
3	HEM	A	404	1,2	-	1/6/54/54	-
4	NHE	A	406	-	-	0/7/15/15	0/1/1/1
4	NHE	B	1406	-	-	2/7/15/15	0/1/1/1
4	NHE	A	407	-	-	0/7/15/15	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	406	NHE	C2-S	-5.35	1.69	1.77
4	B	1406	NHE	C2-S	-5.00	1.70	1.77
4	A	407	NHE	C2-S	-4.23	1.71	1.77
4	B	1407	NHE	C2-S	-4.10	1.71	1.77
3	B	404	HEM	C3C-CAC	-3.78	1.40	1.47
3	A	404	HEM	C3C-CAC	-3.50	1.40	1.47
3	B	404	HEM	CAD-C3D	3.04	1.57	1.52
3	A	404	HEM	CAD-C3D	2.62	1.56	1.52
3	B	404	HEM	C4B-NB	2.57	1.41	1.36
4	A	407	NHE	C1-N	2.43	1.52	1.47
3	A	404	HEM	C4B-NB	2.36	1.41	1.36
3	B	404	HEM	C3B-CAB	-2.28	1.43	1.47
4	B	1407	NHE	C1-N	2.04	1.51	1.47

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	404	HEM	CAA-CBA-CGA	7.58	125.38	112.67
3	A	404	HEM	CAD-CBD-CGD	7.56	125.35	112.67
3	B	404	HEM	CAD-CBD-CGD	7.07	124.53	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	404	HEM	CBD-CAD-C3D	6.79	124.99	112.48
3	A	404	HEM	CBD-CAD-C3D	6.59	124.62	112.48
3	B	404	HEM	CBA-CAA-C2A	6.22	123.95	112.49
3	A	404	HEM	CBA-CAA-C2A	6.10	123.74	112.49
3	A	404	HEM	CAA-CBA-CGA	5.92	122.61	112.67
4	B	1407	NHE	C2-C1-N	-2.74	103.46	111.25
3	B	404	HEM	CMA-C3A-C4A	-2.72	124.28	128.46
3	A	404	HEM	C4C-C3C-C2C	-2.60	105.08	106.90
3	B	404	HEM	C4C-C3C-C2C	-2.58	105.10	106.90
4	A	406	NHE	C2-C1-N	-2.27	104.81	111.25
4	B	1406	NHE	C1-N-C1'	-2.08	110.06	114.14

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1407	NHE	C6'-C1'-N-C1
4	B	1406	NHE	C2'-C1'-N-C1
4	B	1406	NHE	C6'-C1'-N-C1
4	B	1407	NHE	C2'-C1'-N-C1
3	B	404	HEM	C2A-CAA-CBA-CGA
3	A	404	HEM	C2A-CAA-CBA-CGA

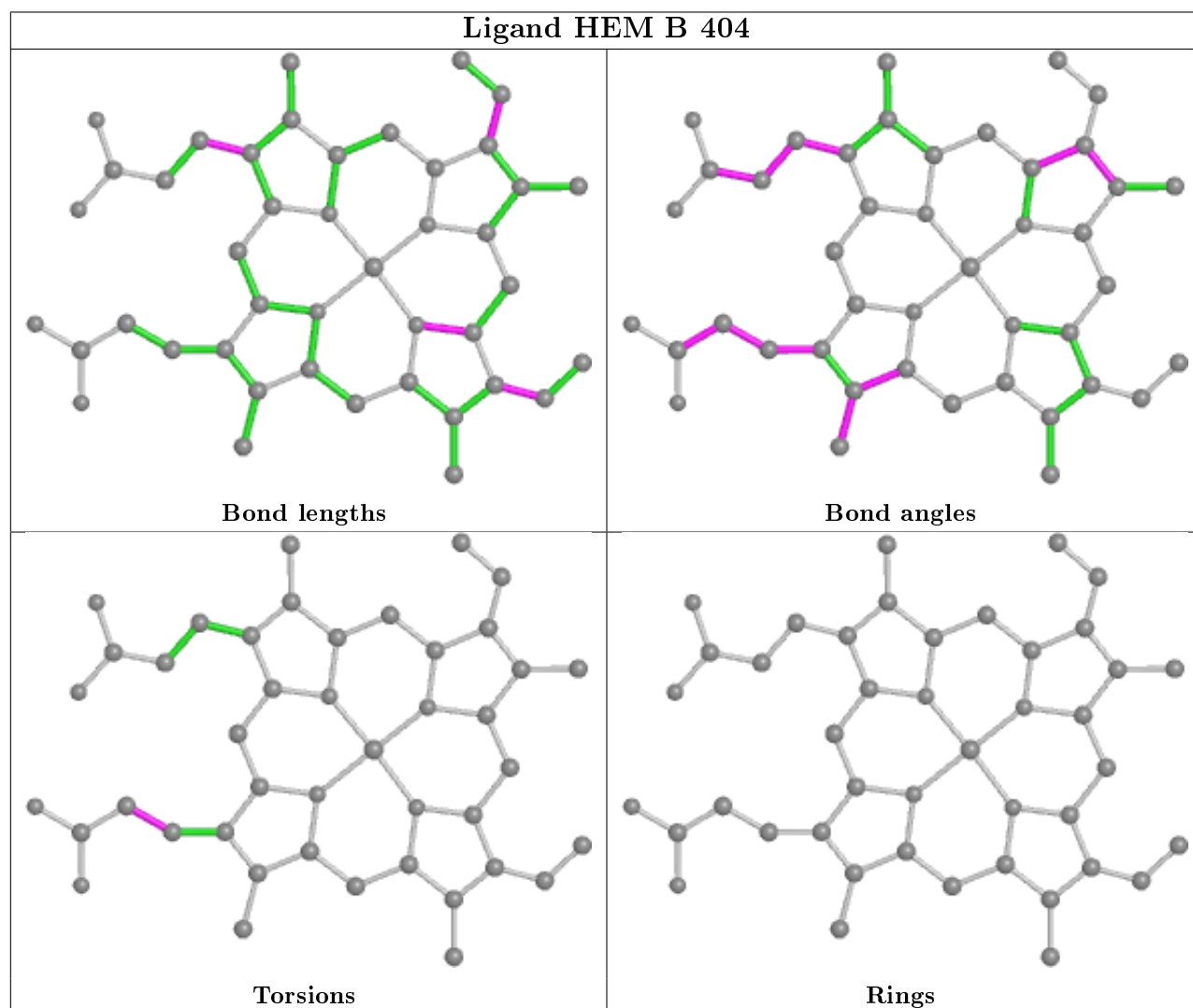
There are no ring outliers.

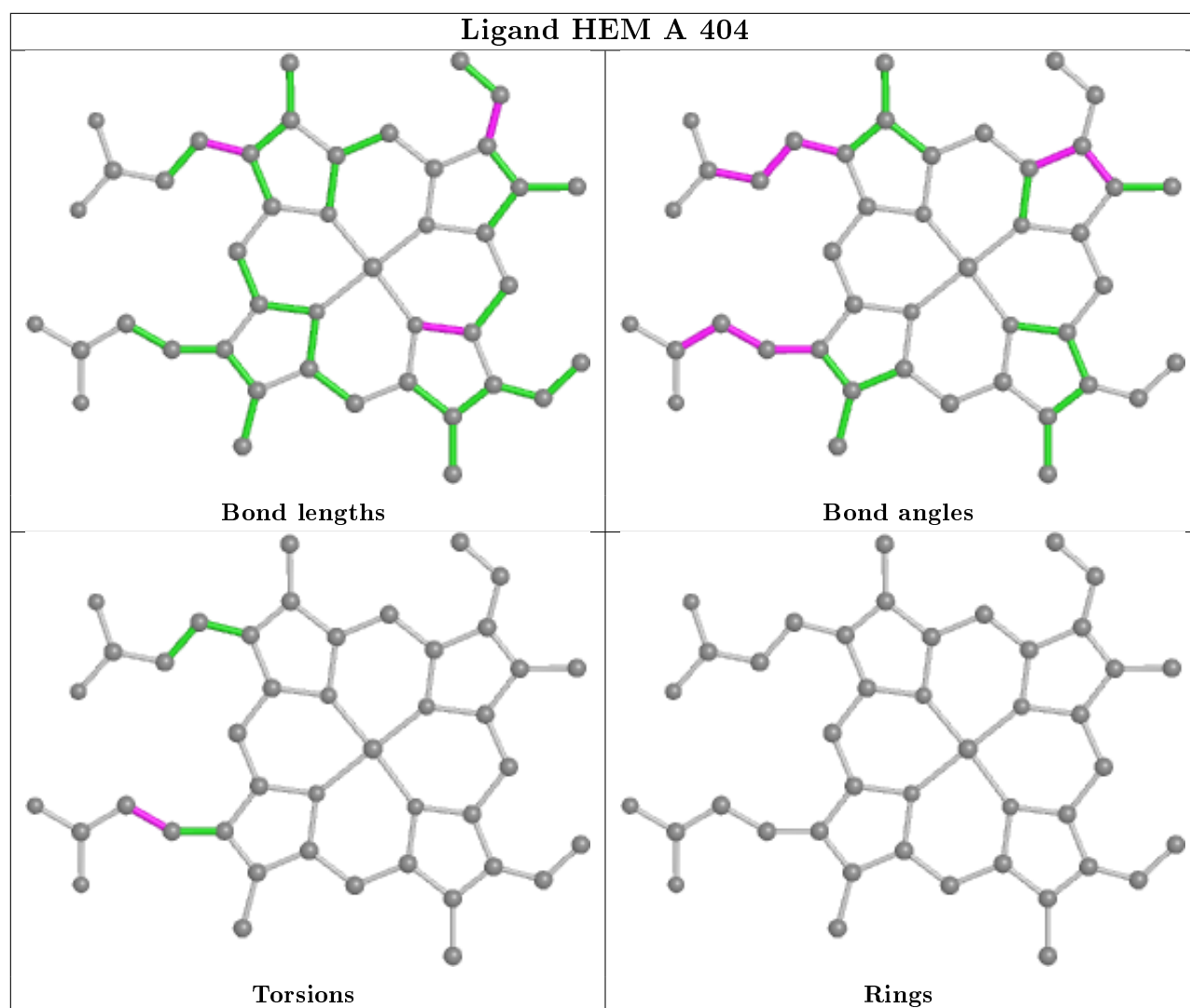
8 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1405	CYN	2	0
4	B	1407	NHE	3	0
3	B	404	HEM	4	0
3	A	404	HEM	4	0
4	A	406	NHE	6	0
4	B	1406	NHE	1	0
4	A	407	NHE	1	0
2	A	405	CYN	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	373/406 (91%)	-0.48	3 (0%) 86 85	13, 41, 81, 100	0
1	B	374/406 (92%)	-0.49	2 (0%) 91 90	16, 42, 85, 100	0
All	All	747/812 (91%)	-0.48	5 (0%) 87 87	13, 42, 82, 100	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	403	GLY	4.6
1	A	402	GLU	3.2
1	B	287	HIS	2.5
1	A	13	LYS	2.3
1	B	11	ILE	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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

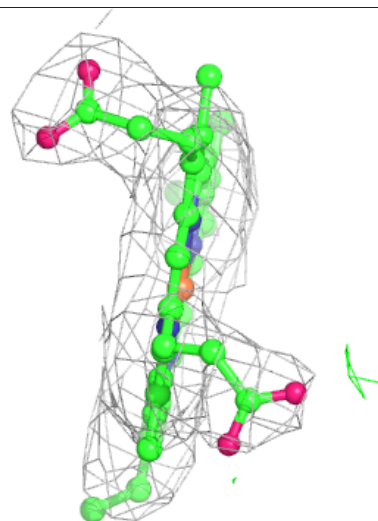
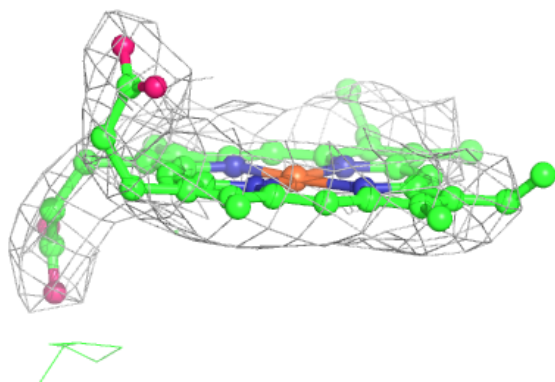
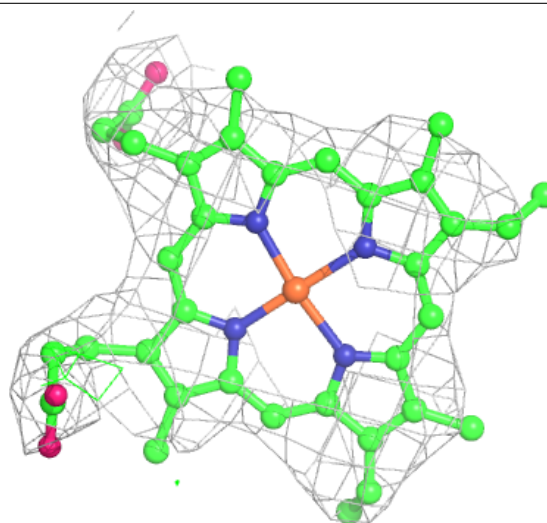
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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	407	13/13	0.77	0.39	82,95,100,100	0
4	NHE	B	1407	13/13	0.84	0.35	70,94,100,100	0
4	NHE	B	1406	13/13	0.89	0.26	51,79,100,100	0
4	NHE	A	406	13/13	0.91	0.25	64,74,94,95	0
3	HEM	B	404	43/43	0.97	0.18	17,27,41,51	0
3	HEM	A	404	43/43	0.98	0.18	15,27,39,54	0
2	CYN	A	405	2/2	0.98	0.22	31,31,31,37	0
2	CYN	B	1405	2/2	0.99	0.22	31,31,31,38	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 404:

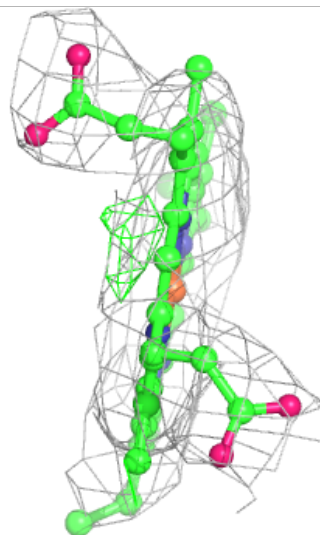
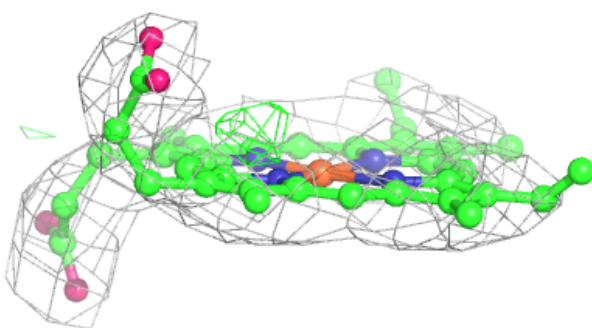
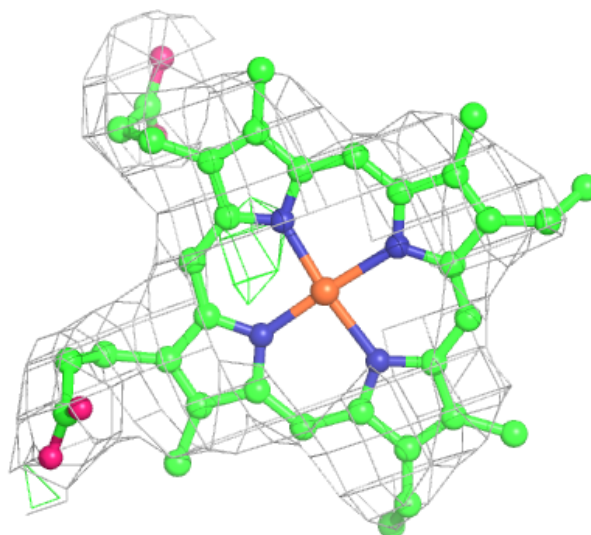
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





**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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.