



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 04:42 am GMT

PDB ID : 1IPH
Title : STRUCTURE OF CATALASE HP11 FROM ESCHERICHIA COLI
Authors : Bravo, J.; Loewen, P.C.; Fita, I.
Deposited on : 1995-12-31
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

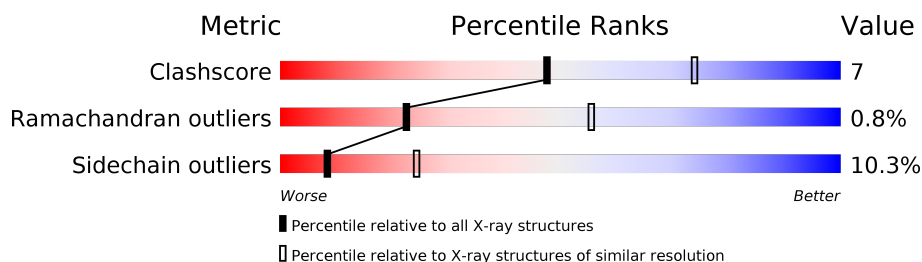
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	753	
1	B	753	
1	C	753	
1	D	753	

2 Entry composition [i](#)

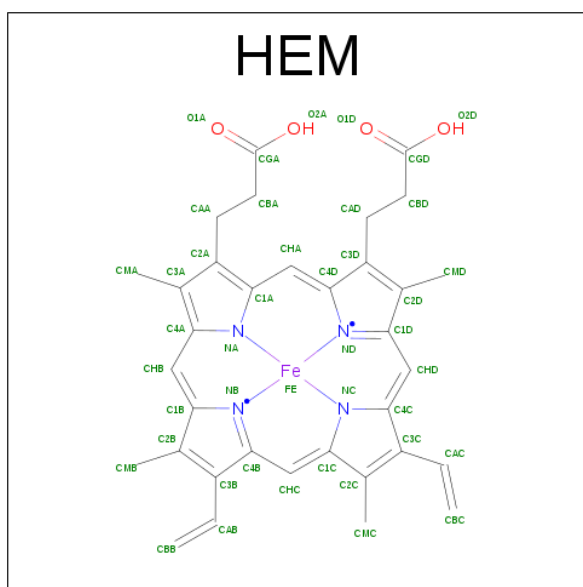
There are 2 unique types of molecules in this entry. The entry contains 23156 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CATALASE HPIL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5746	3647	1005	1082	12			
1	B	727	Total	C	N	O	S	0	0	0
			5746	3647	1005	1082	12			
1	C	727	Total	C	N	O	S	0	0	0
			5746	3647	1005	1082	12			
1	D	727	Total	C	N	O	S	0	0	0
			5746	3647	1005	1082	12			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		
2	B	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		

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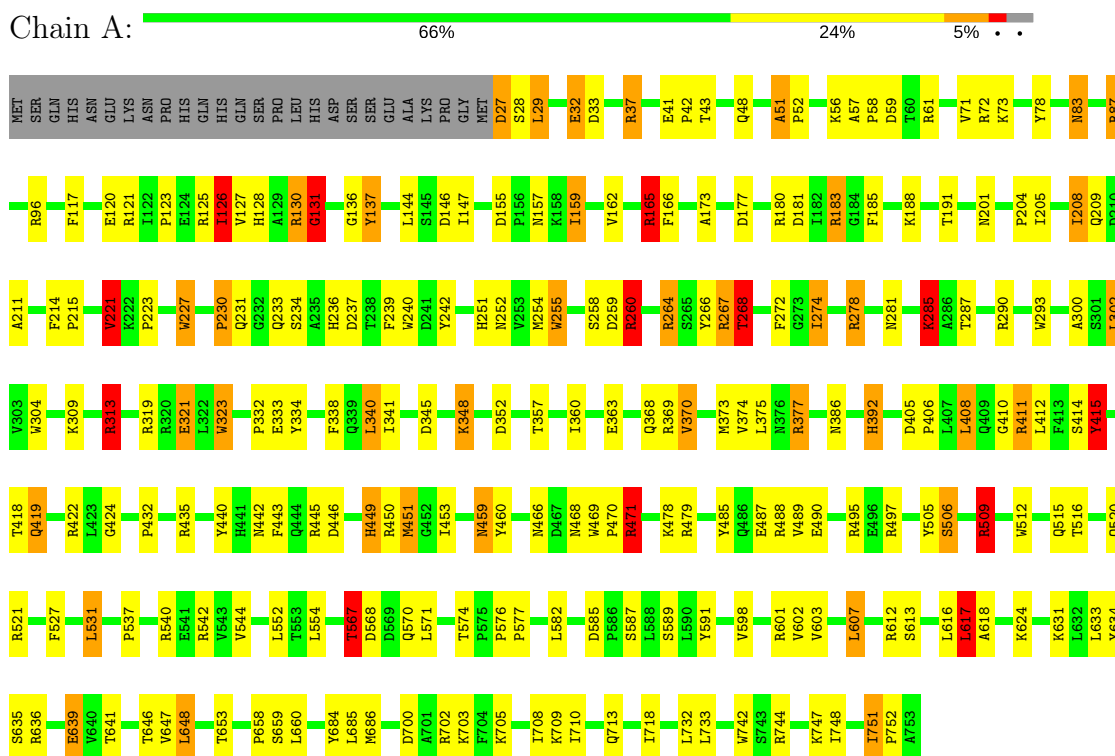
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

3 Residue-property plots

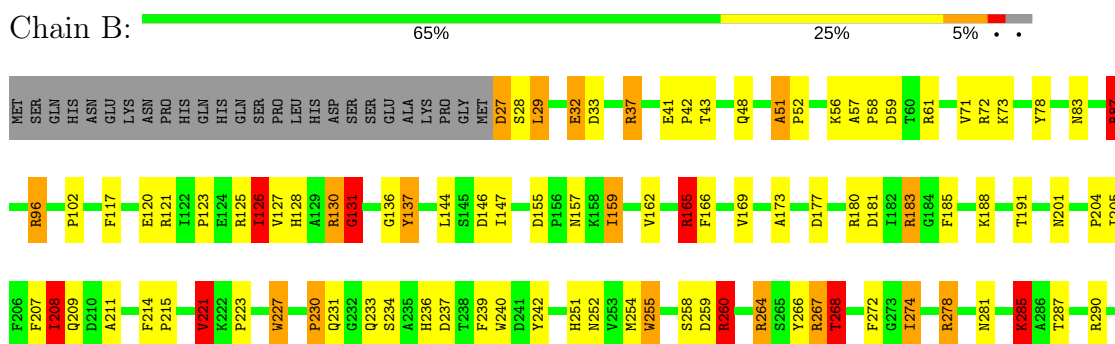
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

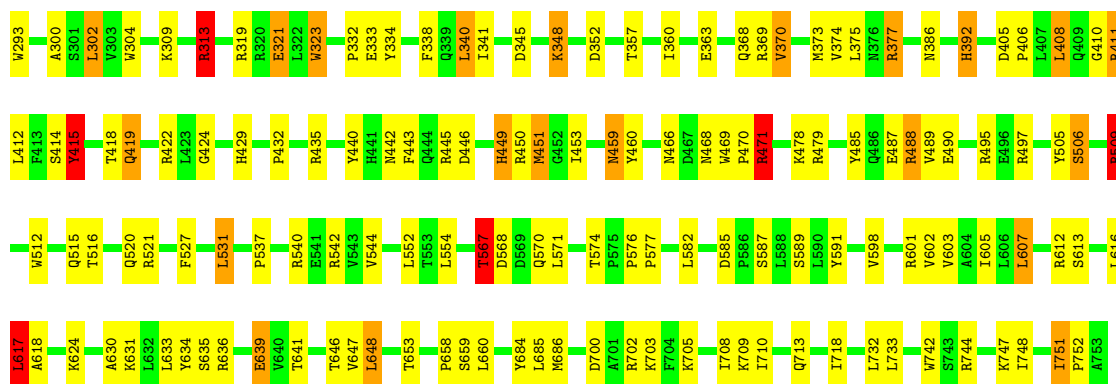
Note EDS was not executed.

• Molecule 1: CATALASE HP11



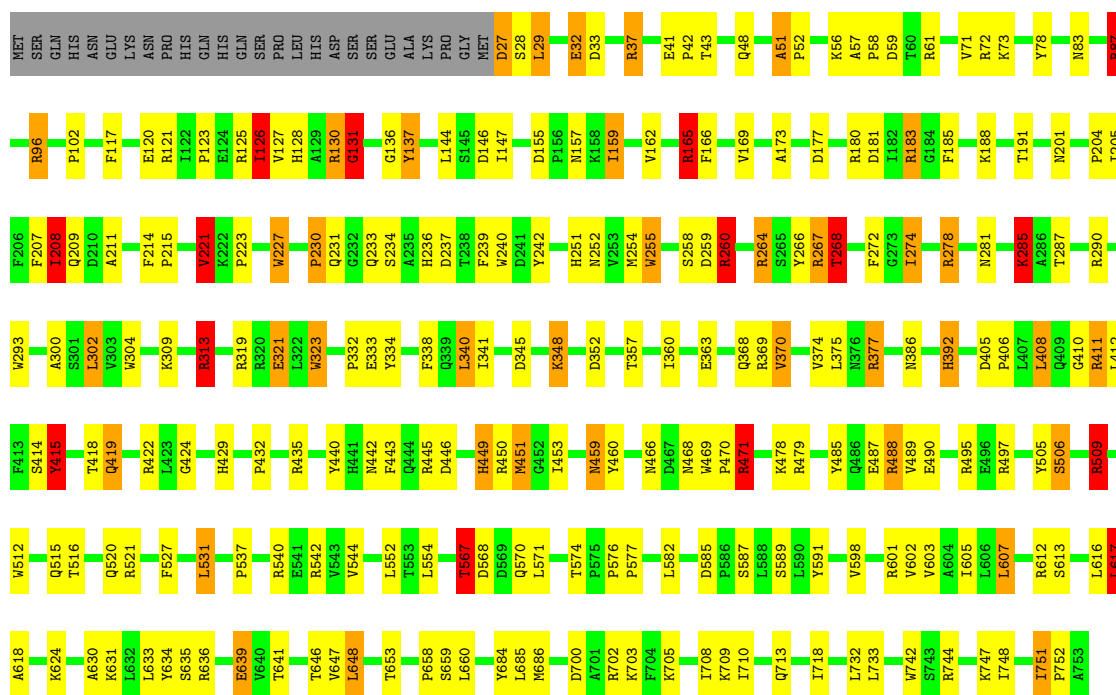
• Molecule 1: CATALASE HP11





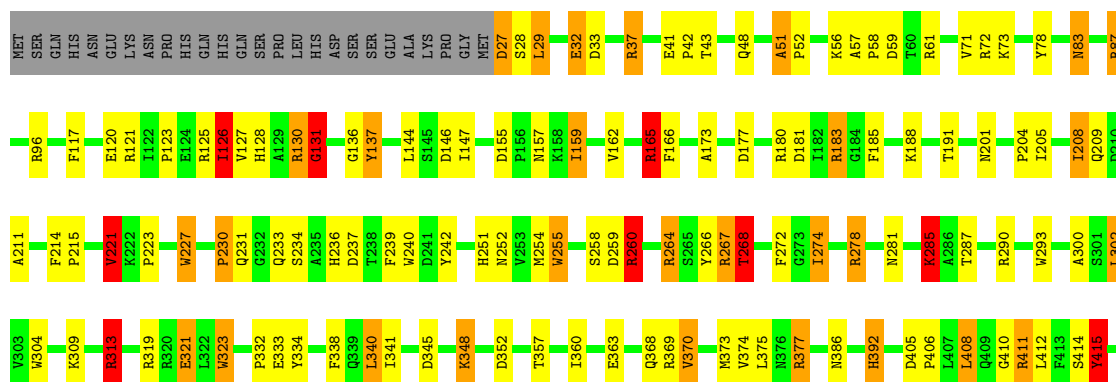
• Molecule 1: CATALASE HPII

Chain C: 65% 25% 5% • •



• Molecule 1: CATALASE HPII

Chain D: 66% 24% 5% • •



S635	R636	E639	V640	T641	T646	V647	L648	T653	P658	S659	L660	Y684	L685	H686	D700	A701	R702	K703	F704	K705	I708	K709	I710	Q713	I718	L732	L733	W742	S743	R744	K747	I748	I751	P752	A753																
R521	F527	L531	P537	R540	E541	R542	V543	V544	L552	T553	L554	T567	D568	D569	Q570	L571	T574	P575	P576	P577	L582	D585	P586	S587	L588	S589	L590	Y591	V598	E598	R601	V602	V603	L607	R612	S613	L616	L617	A618	K624	K631	L632	L633	Y634							
T418	Q419	R422	L423	G424	P432	R435	Y440	H441	H442	F443	Q444	R445	D446	H449	R450	H451	G452	L453	H459	Y460	N466	D467	H468	H469	F470	R471	K478	R479	Y485	Q486	E487	R488	V489	E490	R495	E496	R497	Y505	S506	R509	W512	Q515	T516	L516	L517	A518	K524	K531	L532	L533	Y534

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.20Å 134.70Å 124.40Å 90.00° 109.40° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.200 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	23156	wwPDB-VP
Average B, all atoms (Å ²)	9.0	wwPDB-VP

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: HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.06	7/5902 (0.1%)	1.86	162/8024 (2.0%)
1	B	1.06	7/5902 (0.1%)	1.86	162/8024 (2.0%)
1	C	1.06	7/5902 (0.1%)	1.86	162/8024 (2.0%)
1	D	1.06	7/5902 (0.1%)	1.86	162/8024 (2.0%)
All	All	1.06	28/23608 (0.1%)	1.86	648/32096 (2.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	3
1	D	0	3
All	All	0	12

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	ILE	CA-CB	5.87	1.68	1.54
1	B	208	ILE	CA-CB	5.87	1.68	1.54
1	C	208	ILE	CA-CB	5.87	1.68	1.54
1	D	208	ILE	CA-CB	5.87	1.68	1.54
1	A	449	HIS	CB-CG	5.71	1.60	1.50

The worst 5 of 648 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	ARG	NE-CZ-NH1	17.51	129.05	120.30
1	B	183	ARG	NE-CZ-NH1	17.51	129.05	120.30
1	C	183	ARG	NE-CZ-NH1	17.51	129.05	120.30
1	D	183	ARG	NE-CZ-NH1	17.51	129.05	120.30
1	A	183	ARG	NE-CZ-NH2	-16.87	111.86	120.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	TYR	Sidechain
1	A	415	TYR	Sidechain
1	A	51	ALA	Peptide
1	B	137	TYR	Sidechain
1	B	51	ALA	Peptide

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	5746	0	5578	82	94
1	B	5746	0	5578	88	94
1	C	5746	0	5578	87	94
1	D	5746	0	5578	83	94
2	A	43	0	30	4	0
2	B	43	0	30	3	0
2	C	43	0	30	3	0
2	D	43	0	30	4	0
All	All	23156	0	22432	319	188

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 319 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:392:HIS:CD2	1:A:415:TYR:HB2	2.02	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:HIS:CD2	1:D:415:TYR:HB2	2.02	0.94
1:B:392:HIS:CD2	1:B:415:TYR:HB2	2.02	0.94
1:C:392:HIS:CD2	1:C:415:TYR:HB2	2.02	0.94
1:B:281:ASN:ND2	1:B:285:LYS:HD3	1.95	0.82

The worst 5 of 188 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:59:ASP:CA	1:D:58:PRO:CB[2_555]	0.44	1.76
1:B:58:PRO:CB	1:C:59:ASP:CA[2_545]	0.44	1.76
1:A:58:PRO:CB	1:D:59:ASP:CA[2_555]	0.44	1.76
1:B:59:ASP:CA	1:C:58:PRO:CB[2_545]	0.44	1.76
1:A:59:ASP:OD2	1:D:57:ALA:C[2_555]	0.67	1.53

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	725/753 (96%)	685 (94%)	34 (5%)	6 (1%)	22	55
1	B	725/753 (96%)	685 (94%)	34 (5%)	6 (1%)	22	55
1	C	725/753 (96%)	685 (94%)	34 (5%)	6 (1%)	22	55
1	D	725/753 (96%)	685 (94%)	34 (5%)	6 (1%)	22	55
All	All	2900/3012 (96%)	2740 (94%)	136 (5%)	24 (1%)	22	55

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	B	33	ASP

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Mol	Chain	Res	Type
1	C	33	ASP
1	D	33	ASP
1	A	130	ARG

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	612/636 (96%)	549 (90%)	63 (10%)	8	24
1	B	612/636 (96%)	549 (90%)	63 (10%)	8	24
1	C	612/636 (96%)	549 (90%)	63 (10%)	8	24
1	D	612/636 (96%)	549 (90%)	63 (10%)	8	24
All	All	2448/2544 (96%)	2196 (90%)	252 (10%)	8	24

5 of 252 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	613	SER
1	C	221	VAL
1	D	552	LEU
1	B	639	GLU
1	C	37	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	459	ASN
1	C	368	GLN
1	D	386	ASN
1	B	392	HIS
1	B	449	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
2	HEM	A	754	1	28,50,50	2.08	10 (35%)	17,82,82	2.93	5 (29%)
2	HEM	B	754	1	28,50,50	2.08	10 (35%)	17,82,82	2.93	5 (29%)
2	HEM	C	754	1	28,50,50	2.08	10 (35%)	17,82,82	2.93	5 (29%)
2	HEM	D	754	1	28,50,50	2.08	10 (35%)	17,82,82	2.93	5 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	754	1	-	0/6/54/54	0/0/8/8
2	HEM	B	754	1	-	0/6/54/54	0/0/8/8
2	HEM	C	754	1	-	0/6/54/54	0/0/8/8
2	HEM	D	754	1	-	0/6/54/54	0/0/8/8

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	754	HEM	C3B-CAB	-4.05	1.39	1.47
2	B	754	HEM	C3B-CAB	-4.05	1.39	1.47
2	D	754	HEM	C3B-CAB	-4.05	1.39	1.47
2	A	754	HEM	C3B-CAB	-4.05	1.39	1.47
2	C	754	HEM	C3C-CAC	-3.83	1.40	1.47

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	754	HEM	CBD-CAD-C3D	-10.36	92.71	112.47
2	B	754	HEM	CBD-CAD-C3D	-10.36	92.71	112.47
2	D	754	HEM	CBD-CAD-C3D	-10.36	92.71	112.47
2	A	754	HEM	CBD-CAD-C3D	-10.36	92.71	112.47
2	C	754	HEM	C1D-C2D-C3D	-3.08	104.85	107.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	754	HEM	4	0
2	B	754	HEM	3	0
2	C	754	HEM	3	0
2	D	754	HEM	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.