



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 12:39 PM GMT

PDB ID : 1BE3  
Title : CYTOCHROME BC1 COMPLEX FROM BOVINE  
Authors : Iwata, S.; Lee, J.W.; Okada, K.; Lee, J.K.; Iwata, M.; Ramaswamy, S.; Jap, B.K.  
Deposited on : 1998-05-19  
Resolution : 3.00 Å(reported)

This is a wwPDB validation summary 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 <http://wwpdb.org/ValidationPDFNotes.html>

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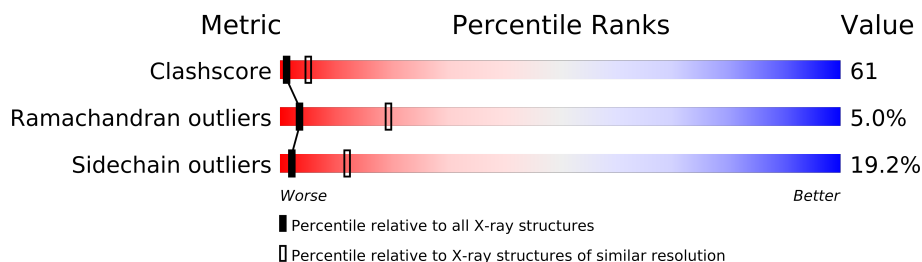
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.00 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	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	446	
2	B	439	
3	C	379	
4	D	241	
5	E	196	
6	F	110	
7	G	81	
8	H	78	
9	I	78	
10	J	62	
11	K	56	

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 16222 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3458	2161	609	668	20			

- Molecule 2 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	419	Total	C	N	O	S	0	0	0
			3141	1972	556	606	7			

- Molecule 3 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	379	Total	C	N	O	S	0	0	0
			3011	2018	472	502	19			

- Molecule 4 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1919	1225	330	349	15			

- Molecule 5 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1519	957	263	291	8			

- Molecule 6 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	106	Total	C	N	O	S	0	0	0
			916	579	166	169	2			

- Molecule 7 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	81	Total	C	N	O	S	0	0	0
			682	441	128	112	1			

- Molecule 8 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	64	Total	C	N	O	S	0	0	0
			524	316	96	107	5			

- Molecule 9 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	33	Total	C	N	O	S	0	0	0
			248	152	51	44	1			

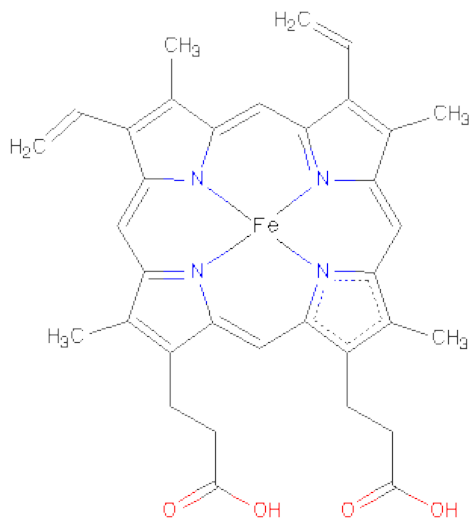
- Molecule 10 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	62	Total	C	N	O		0	0	0
			512	335	89	88				

- Molecule 11 is a protein called CYTOCHROME BC1 COMPLEX.

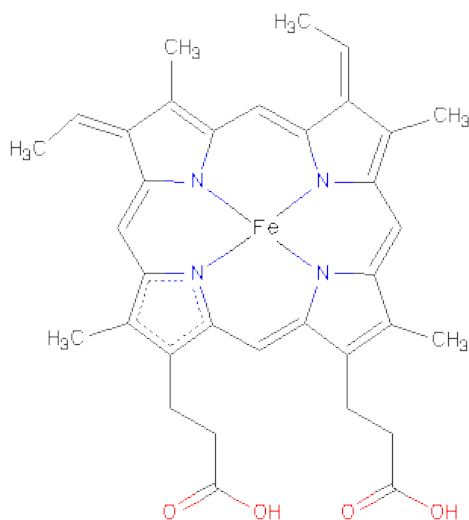
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	22	Total	C	N	O		0	0	0
			159	103	29	27				

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



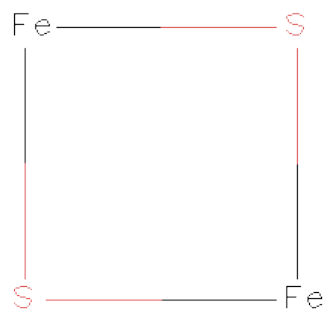
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
12	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

- Molecule 13 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



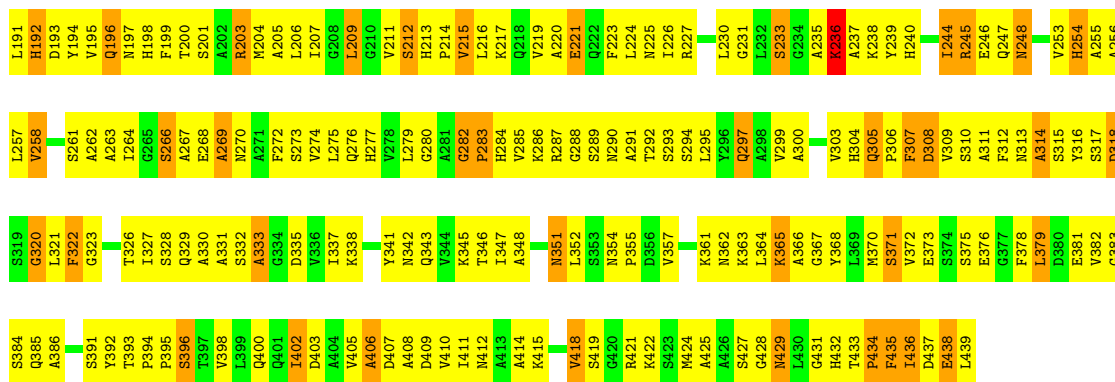
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $Fe_2S_2$ ).



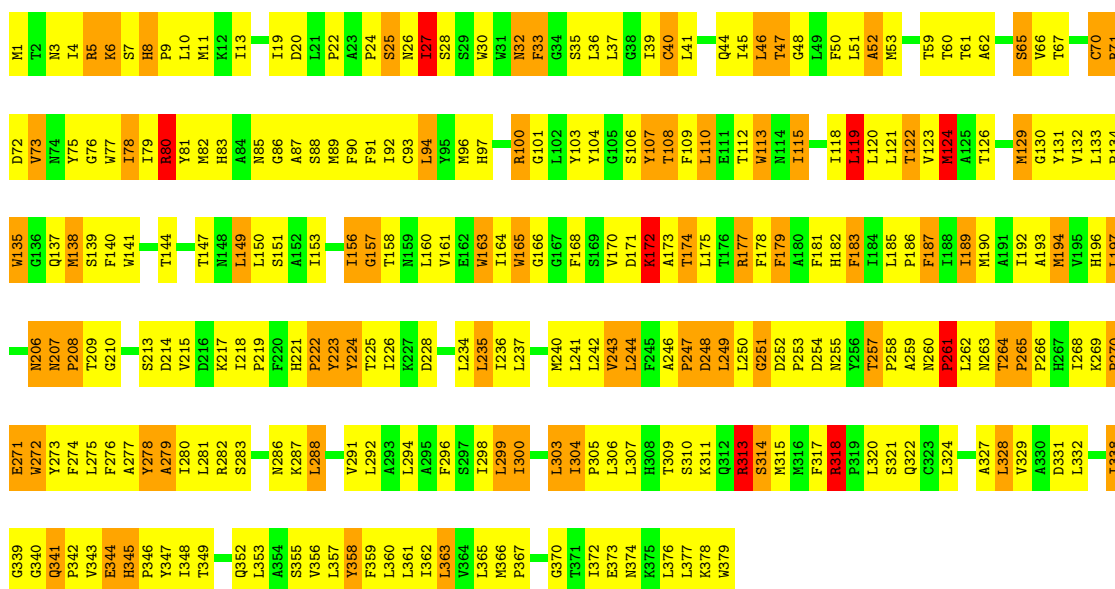
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	E	1	Total	Fe	S	0	0
			4	2	2		





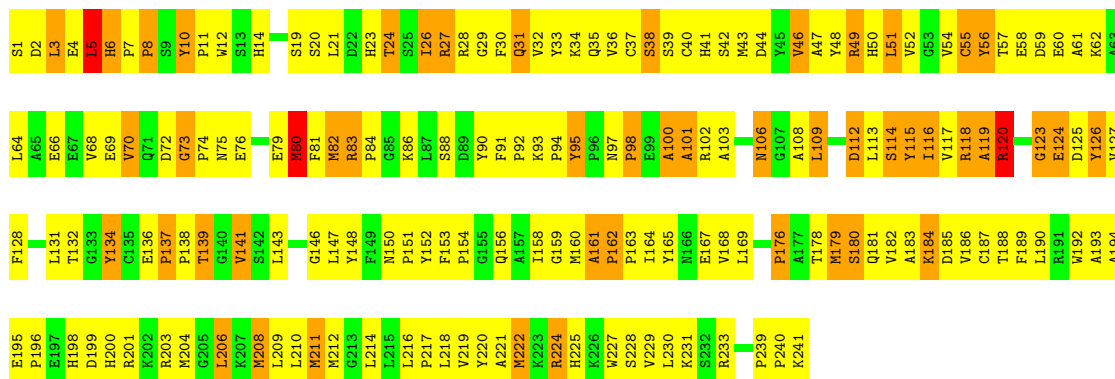
### • Molecule 3: CYTOCHROME BC1 COMPLEX

Chain C:



### • Molecule 4: CYTOCHROME BC1 COMPLEX

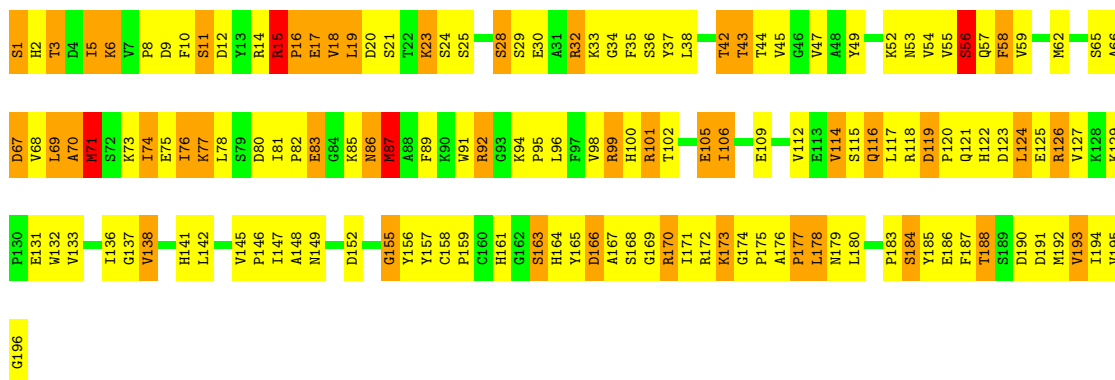
Chain D:



### • Molecule 5: CYTOCHROME BC1 COMPLEX

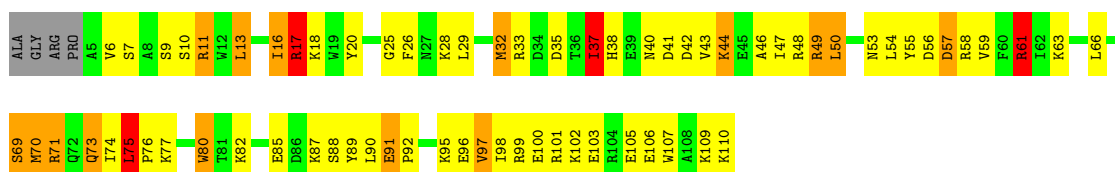
Chain E:





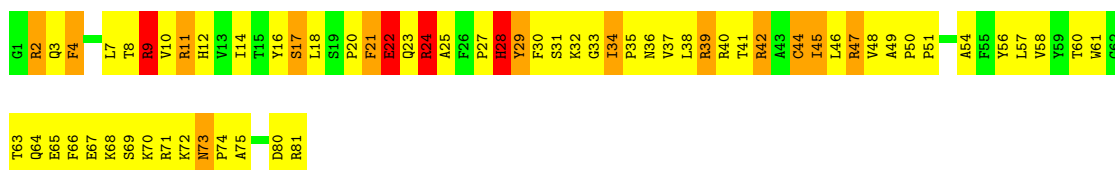
### • Molecule 6: CYTOCHROME BC1 COMPLEX

Chain F:



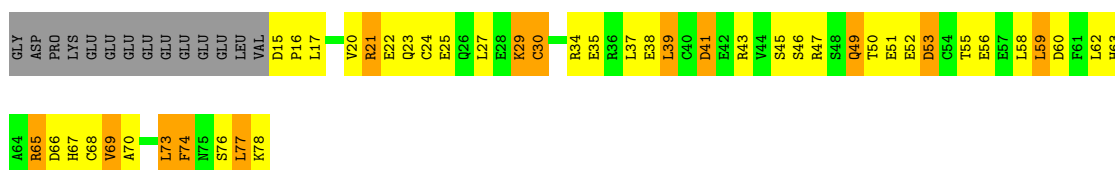
### • Molecule 7: CYTOCHROME BC1 COMPLEX

Chain G:



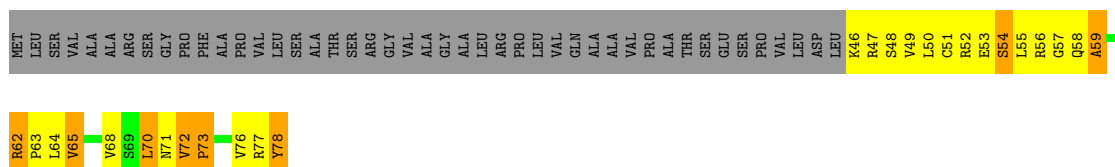
### • Molecule 8: CYTOCHROME BC1 COMPLEX

Chain H:



### • Molecule 9: CYTOCHROME BC1 COMPLEX

Chain I:



### • Molecule 10: CYTOCHROME BC1 COMPLEX

Chain J:



● Molecule 11: CYTOCHROME BC1 COMPLEX

Chain K:

MET	LEU	THR	ARG	PHE	LEU	GLY	PRO	ARG	TYR	ARG	GLN	LEU	ALA	R16	N16	W17	V18	P19	T20	A21	Q22	L23	W24	V30	G31	L32	V33	S34	A35	T36	ASP	SER	ARG	LEU	ILE	LEU	ASP	TRP	VAL	PRO	TYR	ILE	ASN	GLY	LYS	PHE	LYS	LYS	ASP	ASP
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## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.20Å 211.20Å 339.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.00	Depositor
% Data completeness (in resolution range)	81.7 (40.00-3.00)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.260 , 0.320	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16222	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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	0.62	1/3531 (0.0%)	1.63	35/4792 (0.7%)
2	B	0.59	0/3198	1.52	25/4336 (0.6%)
3	C	0.67	2/3108 (0.1%)	1.56	34/4252 (0.8%)
4	D	0.55	0/1978	1.41	15/2684 (0.6%)
5	E	0.55	1/1553 (0.1%)	1.47	16/2100 (0.8%)
6	F	0.58	1/935 (0.1%)	1.59	12/1253 (1.0%)
7	G	0.56	0/704	1.54	11/951 (1.2%)
8	H	0.51	0/529	1.14	1/708 (0.1%)
9	I	0.64	0/250	1.48	1/335 (0.3%)
10	J	0.54	0/525	1.29	4/707 (0.6%)
11	K	0.55	0/163	1.22	1/225 (0.4%)
All	All	0.60	5/16474 (0.0%)	1.52	155/22343 (0.7%)

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	14
2	B	0	17
3	C	0	8
4	D	0	5
5	E	0	5
6	F	0	5
7	G	0	2
8	H	0	1
All	All	0	57

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	344	GLU	CD-OE1	7.85	1.34	1.25
6	F	91	GLU	CD-OE1	7.13	1.33	1.25
3	C	261	PRO	N-CD	-6.11	1.39	1.47
1	A	122	LEU	C-O	5.64	1.34	1.23
5	E	56	SER	C-O	5.41	1.33	1.23

The worst 5 of 155 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	15	ARG	NE-CZ-NH2	15.63	128.11	120.30
3	C	177	ARG	NE-CZ-NH2	-15.12	112.74	120.30
1	A	235	ARG	NE-CZ-NH2	14.30	127.45	120.30
1	A	235	ARG	NE-CZ-NH1	-13.98	113.31	120.30
3	C	80	ARG	NE-CZ-NH1	-13.54	113.53	120.30

There are no chirality outliers.

5 of 57 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	THR	Mainchain
1	A	190	TYR	Mainchain
1	A	197	LEU	Mainchain
1	A	210	ASP	Mainchain
1	A	47	TYR	Mainchain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3458	0	3356	492	0
2	B	3141	0	3123	408	1
3	C	3011	0	3077	382	2
4	D	1919	0	1868	295	0
5	E	1519	0	1503	184	2
6	F	916	0	909	83	0
7	G	682	0	679	104	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	524	0	504	58	0
9	I	248	0	265	76	0
10	J	512	0	518	60	0
11	K	159	0	159	23	0
12	C	86	0	60	19	0
13	D	43	0	30	2	0
14	E	4	0	0	1	0
All	All	16222	0	16051	1980	3

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 61.

The worst 5 of 1980 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:158:PHE:CE1	1:A:317:THR:HG21	1.71	1.26
1:A:21:ASN:CB	1:A:217:SER:HB2	1.70	1.20
1:A:392:LEU:HA	1:A:395:TRP:CD1	1.79	1.17
2:B:29:LEU:HD12	2:B:33:LEU:HD21	1.19	1.15
1:A:158:PHE:HE1	1:A:317:THR:HG21	0.97	1.12

All (3) 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	Distance(Å)	Clash(Å)
3:C:264:THR:OG1	5:E:141:HIS:O[10_665]	1.93	0.27
2:B:169:ARG:NH2	2:B:438:GLU:OE2[10_665]	1.99	0.21
3:C:177:ARG:NH2	5:E:62:MET:O[10_665]	2.12	0.08

## 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	444/446 (100%)	359 (81%)	65 (15%)	20 (4%)	4	22
2	B	417/439 (95%)	360 (86%)	43 (10%)	14 (3%)	6	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	377/379 (100%)	300 (80%)	55 (15%)	22 (6%)	3	15
4	D	239/241 (99%)	188 (79%)	32 (13%)	19 (8%)	1	7
5	E	194/196 (99%)	144 (74%)	40 (21%)	10 (5%)	3	18
6	F	104/110 (94%)	89 (86%)	14 (14%)	1 (1%)	22	70
7	G	79/81 (98%)	57 (72%)	18 (23%)	4 (5%)	3	18
8	H	62/78 (80%)	46 (74%)	11 (18%)	5 (8%)	1	7
9	I	31/78 (40%)	17 (55%)	9 (29%)	5 (16%)	0	1
10	J	60/62 (97%)	47 (78%)	13 (22%)	0	100	100
11	K	20/56 (36%)	15 (75%)	3 (15%)	2 (10%)	1	4
All	All	2027/2166 (94%)	1622 (80%)	303 (15%)	102 (5%)	3	19

5 of 102 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	PRO
1	A	432	PRO
2	B	183	ILE
3	C	8	HIS
3	C	27	ILE

### 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	370/370 (100%)	291 (79%)	79 (21%)	1	8
2	B	328/343 (96%)	265 (81%)	63 (19%)	2	12
3	C	327/327 (100%)	273 (84%)	54 (16%)	3	16
4	D	206/206 (100%)	177 (86%)	29 (14%)	5	23
5	E	168/168 (100%)	124 (74%)	44 (26%)	1	4
6	F	96/98 (98%)	73 (76%)	23 (24%)	1	5
7	G	71/71 (100%)	59 (83%)	12 (17%)	3	15
8	H	61/74 (82%)	52 (85%)	9 (15%)	4	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	27/60 (45%)	21 (78%)	6 (22%)	1	7
10	J	52/52 (100%)	45 (86%)	7 (14%)	6	24
11	K	15/46 (33%)	11 (73%)	4 (27%)	1	4
All	All	1721/1815 (95%)	1391 (81%)	330 (19%)	2	12

5 of 330 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	47	THR
3	C	299	LEU
8	H	21	ARG
3	C	70	CYS
3	C	138	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	329	GLN
3	C	32	ASN
8	H	49	GLN
2	B	343	GLN
3	C	15	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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$
12	HEM	C	380	3	49,50,50	2.26	13 (26%)	46,82,82	1.81	9 (19%)
12	HEM	C	381	3	49,50,50	2.20	11 (22%)	46,82,82	1.77	12 (26%)
13	HEC	D	242	4	50,50,50	2.66	13 (26%)	56,82,82	1.87	16 (28%)
14	FES	E	197	5	0,4,4	0.00	-	0,4,4	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
12	HEM	C	380	3	-	0/14/114/114	0/0/8/8
12	HEM	C	381	3	-	0/14/114/114	0/0/8/8
13	HEC	D	242	4	-	0/10/54/54	0/0/8/8
14	FES	E	197	5	-	0/0/4/4	0/0/1/1

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	242	HEC	C3B-CAB	9.93	1.55	1.35
13	D	242	HEC	C3C-CAC	9.77	1.55	1.35
12	C	381	HEM	C3B-C2B	-6.52	1.32	1.43
12	C	380	HEM	C3B-C2B	-6.17	1.33	1.43
12	C	380	HEM	C3C-C2C	-6.09	1.33	1.43

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	381	HEM	C3B-C4B-NB	-5.28	110.22	114.00
12	C	380	HEM	CMA-C3A-C4A	-5.06	120.83	128.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	380	HEM	C3B-C4B-NB	-4.69	110.65	114.00
13	D	242	HEC	CBC-CAC-C3C	-4.62	115.44	128.44
12	C	380	HEM	CBD-CAD-C3D	4.19	123.52	114.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.