



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:15 am GMT

PDB ID : 2FYU  
Title : Crystal structure of bovine heart mitochondrial bc1 with jg144 inhibitor  
Authors : Xia, D.; Esser, L.  
Deposited on : 2006-02-08  
Resolution : 2.26 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

<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

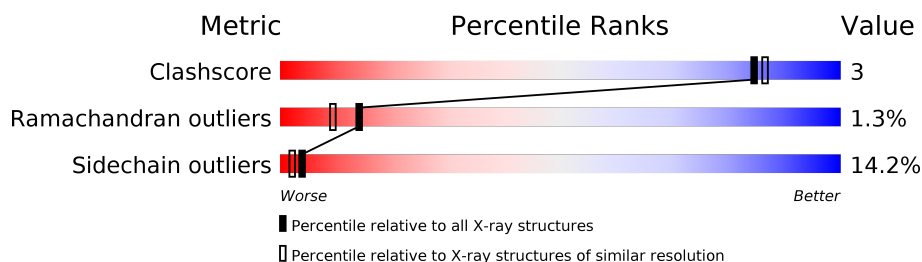
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.26 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	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)

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. 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	446	
2	B	439	
3	C	379	
4	D	241	
5	E	196	
6	F	110	
7	G	81	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	H	78	<div><div></div><div>54%26%18%</div></div>
9	I	78	<div><div></div><div>35%23%12%27%</div></div>
10	J	62	<div><div></div><div>71%24%</div></div>
11	K	56	<div><div></div><div>63%30%5%</div></div>

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 16900 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 Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial.

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 Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	0	0
			3172	1993	562	610	7			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	378	Total	C	N	O	S	0	0	0
			3003	2013	471	501	18			

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1918	1225	330	348	15			

- Molecule 5 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial.

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 Hypothetical protein LOC616871.

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 Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	75	Total	C	N	O	S	0	0	0
			628	410	118	99	1			

- Molecule 8 is a protein called Ubiquinol-cytochrome c reductase complex 11 kDa protein.

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 Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	57	Total	C	N	O	S	0	0	0
			406	253	77	74	2			

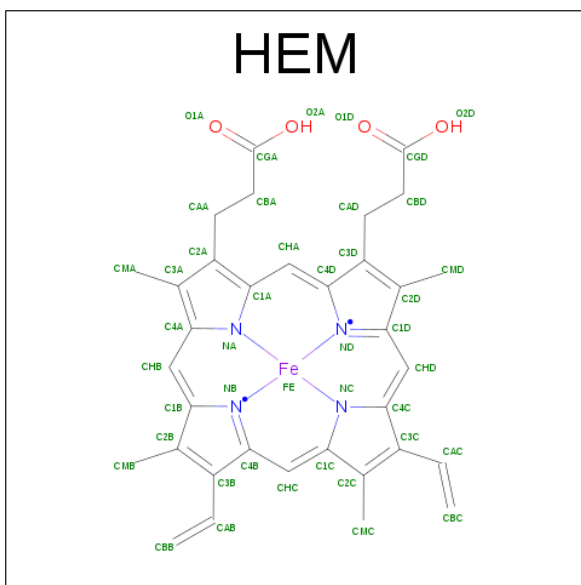
- Molecule 10 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	60	Total	C	N	O	S	0	0	0
			495	324	86	85				

- Molecule 11 is a protein called Ubiquinol-cytochrome c reductase complex 6.4 kDa protein.

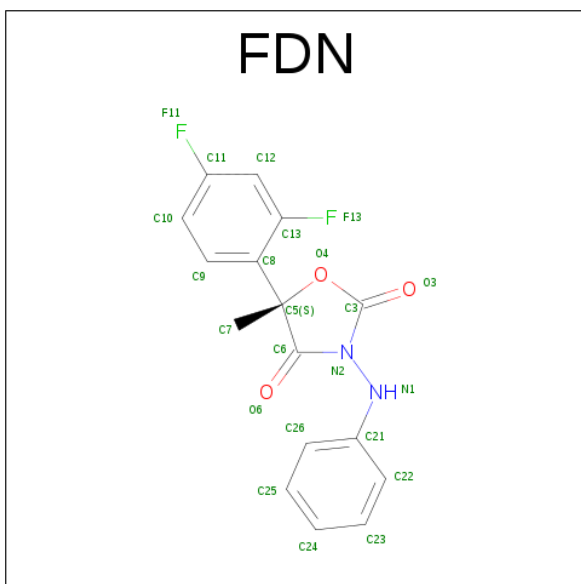
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	53	Total	C	N	O	S	0	0	0
			438	293	78	66	1			

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



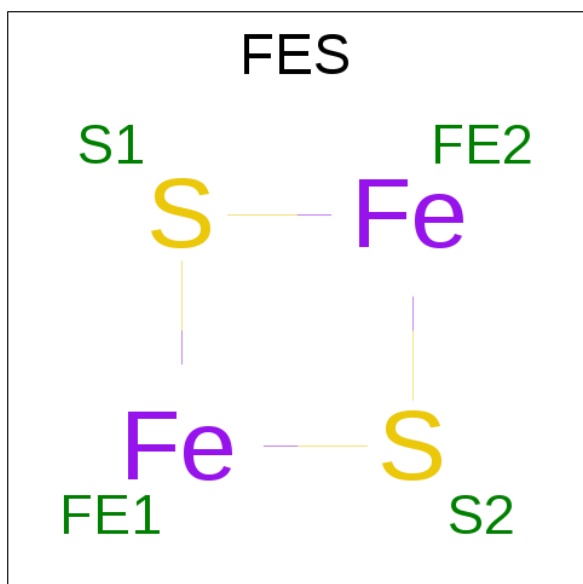
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 13 is (5S)-3-ANILINO-5-(2,4-DIFLUOROPHENYL)-5-METHYL-1,3-OXAZOLIDINE-2,4-DIONE (three-letter code: FDN) (formula:  $C_{16}H_{12}F_2N_2O_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	F	N	O	0	0
			23	16	2	2	3		

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



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

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	38	Total	O	0	0
			38	38		
15	B	53	Total	O	0	0
			53	53		
15	C	84	Total	O	0	0
			84	84		
15	D	34	Total	O	0	0
			34	34		
15	F	27	Total	O	0	0
			27	27		
15	G	13	Total	O	0	0
			13	13		
15	H	2	Total	O	0	0
			2	2		
15	I	6	Total	O	0	0
			6	6		

*Continued on next page...*

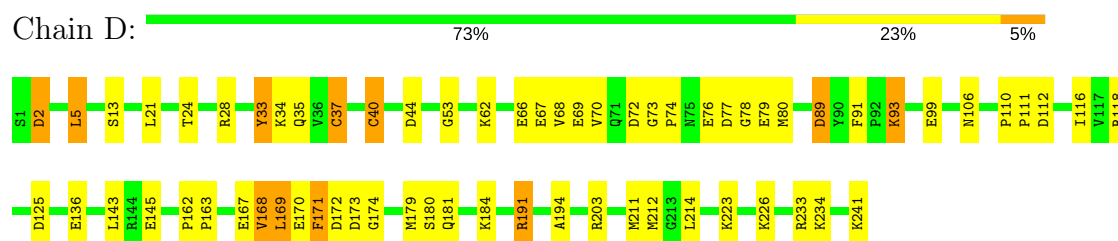
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	J	7	Total	O	0	0
			7	7		
15	K	3	Total	O	0	0
			3	3		

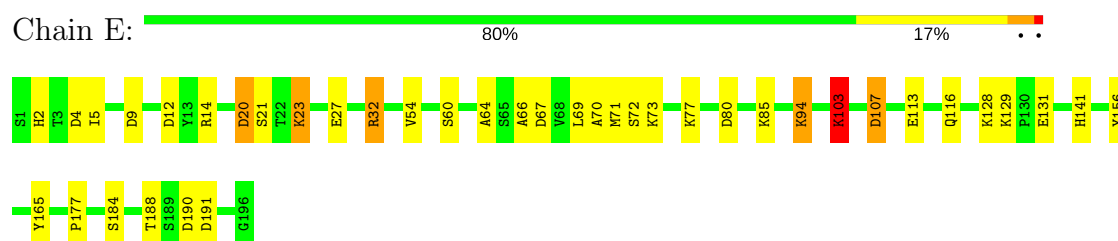




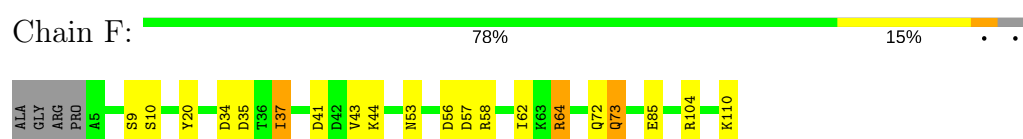
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



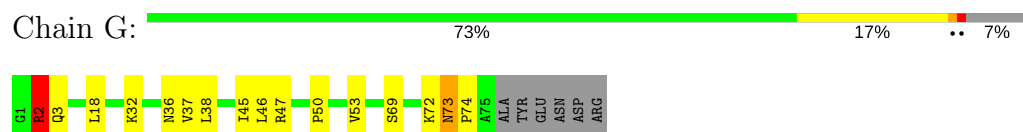
- Molecule 5: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial



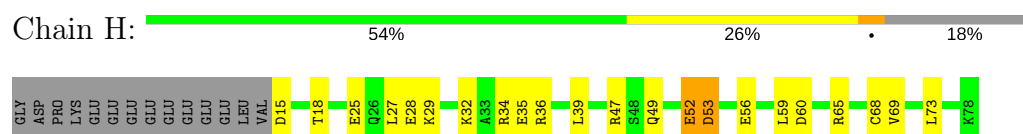
- Molecule 6: Hypothetical protein LOC616871



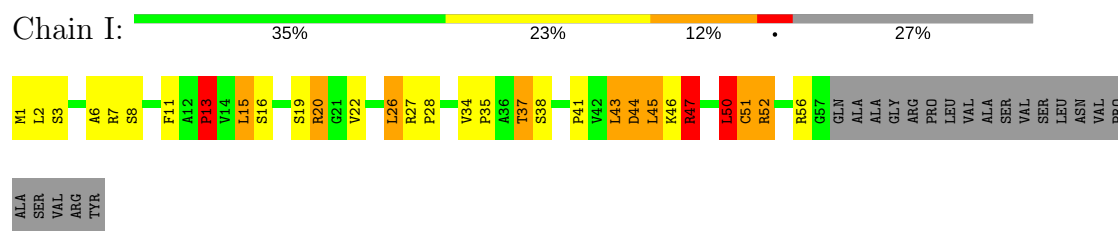
- Molecule 7: Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C



- Molecule 8: Ubiquinol-cytochrome c reductase complex 11 kDa protein



- Molecule 9: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial



- Molecule 10: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

Chain J: 

71%

24%

• •



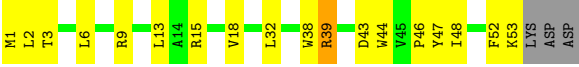
• Molecule 11: Ubiquinol-cytochrome c reductase complex 6.4 kDa protein

Chain K: 

63%

30%

• 5%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.26 Å   154.26 Å   590.19 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	40.00 – 2.26	Depositor
% Data completeness (in resolution range)	96.9 (40.00-2.26)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.248 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16900	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	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, FDN

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	0.97	0/3531	1.06	15/4792 (0.3%)
2	B	1.01	3/3232 (0.1%)	1.04	13/4386 (0.3%)
3	C	1.12	0/3100	1.00	10/4242 (0.2%)
4	D	1.08	0/1977	1.04	11/2684 (0.4%)
5	E	1.07	1/1553 (0.1%)	1.01	8/2100 (0.4%)
6	F	1.09	0/935	1.12	6/1253 (0.5%)
7	G	1.26	0/649	1.07	2/878 (0.2%)
8	H	0.88	0/529	1.07	2/708 (0.3%)
9	I	1.01	0/411	1.24	3/558 (0.5%)
10	J	1.18	0/508	1.02	2/686 (0.3%)
11	K	1.20	0/454	1.02	1/621 (0.2%)
All	All	1.06	4/16879 (0.0%)	1.05	73/22908 (0.3%)

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	12
2	B	0	14
3	C	0	7
4	D	0	9
5	E	0	6
6	F	0	2
8	H	0	1
9	I	0	13
10	J	0	3
11	K	0	4
All	All	0	71

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	103	LYS	CE-NZ	7.62	1.68	1.49
2	B	105	MET	SD-CE	-5.54	1.46	1.77
2	B	272	PHE	CE2-CZ	5.17	1.47	1.37
2	B	57	TYR	CG-CD2	5.05	1.45	1.39

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	245	ARG	NE-CZ-NH2	-8.73	115.93	120.30
6	F	57	ASP	CB-CG-OD2	8.38	125.84	118.30
1	A	244	ARG	NE-CZ-NH2	-8.19	116.21	120.30
1	A	389	ARG	NE-CZ-NH2	-8.13	116.23	120.30
6	F	34	ASP	CB-CG-OD2	7.91	125.42	118.30
4	D	44	ASP	CB-CG-OD2	7.86	125.37	118.30
3	C	20	ASP	CB-CG-OD2	7.80	125.32	118.30
1	A	42	ASP	CB-CG-OD2	7.71	125.24	118.30
2	B	114	ASP	CB-CG-OD2	7.59	125.13	118.30
2	B	407	ASP	CB-CG-OD2	7.44	124.99	118.30
6	F	35	ASP	CB-CG-OD2	7.37	124.93	118.30
1	A	333	ASP	CB-CG-OD2	7.28	124.85	118.30
7	G	2	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	A	142	ASP	CB-CG-OD2	7.19	124.77	118.30
11	K	43	ASP	CB-CG-OD2	7.06	124.65	118.30
5	E	4	ASP	CB-CG-OD2	7.04	124.64	118.30
1	A	370	ASP	CB-CG-OD2	7.01	124.61	118.30
6	F	56	ASP	CB-CG-OD2	6.99	124.59	118.30
2	B	356	ASP	CB-CG-OD2	6.96	124.57	118.30
2	B	335	ASP	CB-CG-OD2	6.94	124.55	118.30
8	H	15	ASP	CB-CG-OD2	6.92	124.53	118.30
2	B	23	ASP	CB-CG-OD2	6.90	124.51	118.30
4	D	125	ASP	CB-CG-OD2	6.78	124.40	118.30
6	F	41	ASP	CB-CG-OD2	6.65	124.29	118.30
2	B	380	ASP	CB-CG-OD2	6.56	124.21	118.30
2	B	308	ASP	CB-CG-OD2	6.56	124.20	118.30
10	J	36	ASP	CB-CG-OD2	6.55	124.19	118.30
3	C	214	ASP	CB-CG-OD2	6.47	124.12	118.30
9	I	43	LEU	CA-CB-CG	6.46	130.17	115.30
2	B	318	ASP	CB-CG-OD2	6.46	124.11	118.30
2	B	403	ASP	CB-CG-OD2	6.42	124.08	118.30
4	D	173	ASP	CB-CG-OD2	6.41	124.07	118.30
5	E	9	ASP	CB-CG-OD2	6.24	123.92	118.30
1	A	23	LEU	CA-CB-CG	6.15	129.45	115.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	ASP	CB-CG-OD2	6.08	123.77	118.30
5	E	20	ASP	CB-CG-OD2	5.97	123.67	118.30
3	C	361	LEU	CA-CB-CG	5.86	128.79	115.30
5	E	32	ARG	NE-CZ-NH2	-5.82	117.39	120.30
5	E	191	ASP	CB-CG-OD2	5.81	123.53	118.30
4	D	72	ASP	CB-CG-OD2	5.81	123.53	118.30
3	C	248	ASP	CB-CG-OD2	5.76	123.49	118.30
3	C	94	LEU	CA-CB-CG	5.76	128.55	115.30
1	A	124	ASP	CB-CG-OD2	5.75	123.48	118.30
7	G	2	ARG	NE-CZ-NH2	-5.73	117.43	120.30
2	B	257	LEU	CB-CG-CD2	5.67	120.65	111.00
4	D	77	ASP	CB-CG-OD2	5.64	123.37	118.30
1	A	327	ASP	CB-CG-OD2	5.55	123.30	118.30
3	C	94	LEU	CB-CG-CD1	5.50	120.34	111.00
4	D	233	ARG	NE-CZ-NH2	-5.48	117.56	120.30
8	H	53	ASP	CB-CG-OD2	5.45	123.21	118.30
1	A	438	ARG	NE-CZ-NH2	-5.45	117.58	120.30
4	D	233	ARG	NE-CZ-NH1	5.44	123.02	120.30
4	D	89	ASP	CB-CG-OD2	5.42	123.17	118.30
5	E	107	ASP	CB-CG-OD2	5.35	123.11	118.30
2	B	387	LEU	CB-CG-CD1	5.32	120.05	111.00
1	A	210	ASP	CB-CG-OD2	5.31	123.08	118.30
3	C	318	ARG	NE-CZ-NH2	-5.30	117.65	120.30
9	I	15	LEU	CA-CB-CG	5.30	127.49	115.30
10	J	51	LEU	CA-CB-CG	5.29	127.46	115.30
4	D	2	ASP	CB-CG-OD2	5.28	123.05	118.30
3	C	318	ARG	NE-CZ-NH1	5.28	122.94	120.30
4	D	172	ASP	CB-CG-OD2	5.28	123.05	118.30
5	E	80	ASP	CB-CG-OD2	5.27	123.05	118.30
3	C	254	ASP	CB-CG-OD2	5.24	123.02	118.30
4	D	112	ASP	CB-CG-OD2	5.23	123.01	118.30
5	E	190	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	20	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	388	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	281	ASP	CB-CG-OD1	-5.19	113.63	118.30
3	C	331	ASP	CB-CG-OD2	5.14	122.93	118.30
6	F	104	ARG	NE-CZ-NH2	-5.07	117.77	120.30
9	I	44	ASP	CB-CG-OD2	5.04	122.84	118.30
2	B	147	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

All (71) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	20	ASP	Peptide
1	A	227	ALA	Peptide
1	A	228	VAL	Peptide
1	A	229	PRO	Peptide
1	A	244	ARG	Sidechain
1	A	278	GLY	Mainchain
1	A	281	ASP	Sidechain
1	A	303	LEU	Peptide
1	A	389	ARG	Sidechain
1	A	402	VAL	Mainchain
1	A	408	ARG	Sidechain
1	A	48	GLU	Mainchain
2	B	149	ALA	Mainchain
2	B	169	ARG	Peptide
2	B	17	VAL	Peptide
2	B	170	ASN	Peptide
2	B	171	ALA	Mainchain
2	B	18	PRO	Peptide
2	B	226	ILE	Peptide
2	B	227	ARG	Peptide
2	B	231	GLY	Peptide
2	B	234	GLY	Peptide
2	B	245	ARG	Sidechain
2	B	249	GLY	Peptide
2	B	322	PHE	Sidechain
2	B	434	PRO	Mainchain
3	C	139	SER	Mainchain
3	C	22	PRO	Mainchain
3	C	264	THR	Peptide
3	C	344	GLU	Peptide
3	C	346	PRO	Mainchain
3	C	5	ARG	Sidechain
3	C	71	ARG	Sidechain
4	D	145	GLU	Peptide
4	D	162	PRO	Mainchain
4	D	163	PRO	Peptide
4	D	33	TYR	Sidechain
4	D	53	GLY	Peptide
4	D	70	VAL	Peptide
4	D	73	GLY	Peptide
4	D	78	GLY	Peptide
4	D	91	PHE	Peptide
5	E	14	ARG	Sidechain

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Group
5	E	32	ARG	Sidechain
5	E	64	ALA	Mainchain
5	E	66	ALA	Peptide
5	E	70	ALA	Peptide
5	E	94	LYS	Peptide
6	F	20	TYR	Sidechain
6	F	73	GLN	Mainchain
8	H	52	GLU	Peptide
9	I	13	PRO	Mainchain
9	I	26	LEU	Peptide
9	I	34	VAL	Peptide
9	I	35	PRO	Peptide
9	I	37	THR	Peptide
9	I	43	LEU	Peptide
9	I	45	LEU	Peptide
9	I	46	LYS	Peptide
9	I	47	ARG	Mainchain
9	I	50	LEU	Mainchain,Peptide
9	I	52	ARG	Peptide
9	I	6	ALA	Peptide
10	J	2	ALA	Peptide
10	J	50	LYS	Peptide
10	J	51	LEU	Peptide
11	K	38	TRP	Mainchain,Peptide
11	K	46	PRO	Peptide
11	K	47	TYR	Peptide

## 5.2 Too-close contacts [i](#)

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	3458	0	3356	17	0
2	B	3172	0	3152	22	0
3	C	3003	0	3065	22	0
4	D	1918	0	1870	13	0
5	E	1519	0	1503	9	0
6	F	916	0	909	3	0
7	G	628	0	636	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	524	0	504	2	0
9	I	406	0	437	5	0
10	J	495	0	493	2	0
11	K	438	0	447	2	0
12	C	86	0	60	2	0
12	D	43	0	30	2	0
13	C	23	0	12	1	0
14	E	4	0	0	0	0
15	A	38	0	0	0	0
15	B	53	0	0	1	0
15	C	84	0	0	0	0
15	D	34	0	0	0	0
15	F	27	0	0	0	0
15	G	13	0	0	0	0
15	H	2	0	0	0	0
15	I	6	0	0	0	0
15	J	7	0	0	0	0
15	K	3	0	0	0	0
All	All	16900	0	16474	89	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (89) 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)
5:E:103:LYS:CE	5:E:103:LYS:NZ	1.68	1.53
2:B:385:GLN:HE22	2:B:393:THR:H	1.22	0.88
3:C:217:LYS:HE3	7:G:2:ARG:HH22	1.48	0.76
3:C:45:ILE:HA	12:C:381:HEM:HAB	1.73	0.70
2:B:248:ASN:HB3	2:B:250:ASP:HB2	1.79	0.65
5:E:103:LYS:HE3	5:E:107:ASP:OD2	1.98	0.62
2:B:76:THR:HG23	2:B:81:SER:HA	1.81	0.62
1:A:255:ILE:HG21	1:A:335:MET:HE1	1.83	0.61
2:B:308:ASP:OD1	9:I:28:PRO:HB2	2.01	0.61
3:C:214:ASP:OD2	7:G:2:ARG:NH2	2.34	0.60
6:F:64:ARG:HH11	6:F:64:ARG:HB3	1.68	0.59
5:E:103:LYS:NZ	5:E:103:LYS:CD	2.63	0.58
1:A:48:GLU:HB2	1:A:52:ASN:HB3	1.85	0.58
2:B:385:GLN:HE22	2:B:393:THR:N	1.98	0.55
4:D:74:PRO:HB3	4:D:79:GLU:H	1.72	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:309:THR:HG21	3:C:367:PRO:O	2.07	0.54
1:A:19:LEU:HB3	1:A:21:ASN:HB2	1.89	0.54
3:C:349:THR:HA	3:C:352:GLN:HE21	1.73	0.53
15:B:482:HOH:O	9:I:15:LEU:HD12	2.08	0.53
5:E:156:TYR:HB2	5:E:165:TYR:HB2	1.90	0.53
4:D:118:ARG:HG3	4:D:194:ALA:HB1	1.91	0.53
2:B:357:VAL:HG12	2:B:361:LYS:HD2	1.92	0.52
2:B:169:ARG:HG3	2:B:240:HIS:HB2	1.93	0.51
3:C:275:LEU:HB2	3:C:336:THR:HG22	1.93	0.51
1:A:48:GLU:HG3	1:A:53:ASN:HA	1.93	0.50
6:F:37:ILE:HD12	6:F:43:VAL:HG21	1.93	0.50
2:B:258:VAL:HG12	2:B:423:SER:HB2	1.93	0.50
6:F:58:ARG:O	6:F:62:ILE:HG12	2.11	0.50
5:E:20:ASP:HB3	5:E:23:LYS:HB2	1.94	0.50
1:A:45:SER:HA	1:A:48:GLU:HG2	1.92	0.49
3:C:268:ILE:HG23	13:C:400:FDN:H25	1.94	0.49
4:D:37:CYS:SG	12:D:242:HEM:HAB	2.53	0.49
2:B:309:VAL:HG13	2:B:326:THR:HG22	1.95	0.49
7:G:50:PRO:HA	7:G:53:VAL:HG22	1.94	0.48
4:D:21:LEU:HD21	4:D:191:ARG:HG2	1.96	0.48
11:K:3:THR:HA	11:K:6:LEU:HD12	1.96	0.48
2:B:95:LYS:HB2	2:B:110:GLU:HG2	1.95	0.47
3:C:237:LEU:HD13	4:D:212:MET:HG2	1.95	0.47
4:D:171:PHE:HB3	4:D:174:GLY:HA2	1.97	0.47
1:A:146:ARG:HE	1:A:308:GLN:HE22	1.63	0.47
2:B:100:SER:O	9:I:13:PRO:HD2	2.16	0.46
3:C:150:LEU:HB2	3:C:161:VAL:HG22	1.97	0.46
2:B:37:SER:HB3	2:B:216:LEU:HD12	1.97	0.46
3:C:8:HIS:HD2	3:C:11:MET:H	1.64	0.46
3:C:287:LYS:HG2	5:E:141:HIS:HD2	1.81	0.46
3:C:206:ASN:HD21	3:C:210:GLY:HA2	1.81	0.45
1:A:308:GLN:HE21	1:A:323:HIS:CD2	2.35	0.45
1:A:102:LEU:HD23	1:A:104:LYS:HE3	1.99	0.45
2:B:385:GLN:NE2	2:B:393:THR:H	2.02	0.45
3:C:322:GLN:NE2	7:G:47:ARG:HH11	2.15	0.45
3:C:246:ALA:HB1	3:C:249:LEU:HB2	1.99	0.44
3:C:287:LYS:HG3	5:E:177:PRO:HD3	1.99	0.44
10:J:33:ARG:HD3	11:K:48:ILE:HA	1.99	0.44
3:C:101:GLY:HA2	3:C:106:SER:HB2	1.99	0.44
1:A:39:VAL:HG11	1:A:117:VAL:HG21	2.00	0.43
3:C:58:ASP:HB3	3:C:61:THR:HG22	1.99	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:LYS:HB2	2:B:203:ARG:HB3	2.00	0.43
2:B:264:ILE:HG12	9:I:2:LEU:HD23	1.99	0.43
4:D:28:ARG:HD3	4:D:171:PHE:HE2	1.84	0.43
7:G:45:ILE:HD12	7:G:46:LEU:HG	2.01	0.43
1:A:346:CYS:O	1:A:408:ARG:HB2	2.19	0.43
4:D:33:TYR:HA	4:D:37:CYS:SG	2.59	0.43
2:B:141:GLN:NE2	2:B:186:VAL:O	2.51	0.43
9:I:20:ARG:HG2	9:I:20:ARG:H	1.58	0.43
3:C:44:GLN:HG3	12:C:381:HEM:HBC2	2.00	0.43
2:B:200:THR:HB	2:B:227:ARG:HG2	2.00	0.43
2:B:78:LYS:HB2	2:B:129:ALA:HB1	2.00	0.42
3:C:287:LYS:HE2	5:E:177:PRO:HG3	2.02	0.42
3:C:15:ASN:HA	3:C:19:ILE:HG12	2.01	0.42
4:D:5:LEU:HB3	8:H:59:LEU:HD22	2.02	0.42
2:B:436:ILE:HA	2:B:439:LEU:HD12	2.01	0.42
1:A:21:ASN:HD21	1:A:217:SER:HA	1.85	0.42
5:E:2:HIS:HA	5:E:5:ILE:HD12	2.01	0.42
1:A:79:VAL:HG21	1:A:86:LEU:HD22	2.01	0.42
4:D:211:MET:HE2	4:D:211:MET:HA	2.02	0.42
4:D:40:CYS:SG	12:D:242:HEM:HAC	2.60	0.42
1:A:27:SER:HB3	1:A:208:LEU:HD12	2.02	0.41
2:B:109:VAL:HG22	2:B:119:LEU:HD12	2.02	0.41
1:A:361:LEU:HD23	1:A:399:ILE:HG12	2.02	0.41
1:A:60:GLU:OE2	2:B:287:ARG:NH2	2.53	0.41
4:D:110:PRO:HA	4:D:111:PRO:HD3	1.94	0.41
10:J:10:TYR:HA	10:J:14:PHE:HB2	2.03	0.41
1:A:252:HIS:CD2	1:A:323:HIS:HE1	2.39	0.41
2:B:209:LEU:HD13	2:B:379:LEU:HD12	2.02	0.41
4:D:168:VAL:HB	4:D:169:LEU:HD12	2.03	0.41
1:A:298:ALA:HB1	1:A:304:CYS:HB2	2.03	0.41
3:C:173:ALA:O	3:C:177:ARG:HB2	2.20	0.40
8:H:69:VAL:HG13	8:H:73:LEU:HD13	2.04	0.40
3:C:177:ARG:HG2	3:C:181:PHE:CE2	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	444/446 (100%)	427 (96%)	12 (3%)	5 (1%)	17	12
2	B	421/439 (96%)	396 (94%)	22 (5%)	3 (1%)	25	25
3	C	376/379 (99%)	356 (95%)	18 (5%)	2 (0%)	32	33
4	D	239/241 (99%)	215 (90%)	21 (9%)	3 (1%)	14	9
5	E	194/196 (99%)	183 (94%)	8 (4%)	3 (2%)	12	7
6	F	104/110 (94%)	102 (98%)	2 (2%)	0	100	100
7	G	73/81 (90%)	68 (93%)	3 (4%)	2 (3%)	6	3
8	H	62/78 (80%)	60 (97%)	2 (3%)	0	100	100
9	I	55/78 (70%)	36 (66%)	11 (20%)	8 (14%)	0	0
10	J	58/62 (94%)	51 (88%)	7 (12%)	0	100	100
11	K	51/56 (91%)	45 (88%)	4 (8%)	2 (4%)	3	1
All	All	2077/2166 (96%)	1939 (93%)	110 (5%)	28 (1%)	14	9

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
1	A	224	ASP
2	B	437	ASP
3	C	29	SER
5	E	67	ASP
5	E	73	LYS
7	G	73	ASN
9	I	3	SER
9	I	47	ARG
9	I	51	CYS
11	K	39	ARG
1	A	21	ASN
1	A	262	TRP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	D	80	MET
5	E	72	SER
11	K	52	PHE
1	A	227	ALA
4	D	93	LYS
9	I	41	PRO
9	I	44	ASP
9	I	45	LEU
9	I	50	LEU
2	B	236	LYS
3	C	268	ILE
4	D	169	LEU
2	B	436	ILE
7	G	74	PRO
9	I	13	PRO

### 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%)	325 (88%)	45 (12%)	6	4
2	B	332/343 (97%)	297 (90%)	35 (10%)	8	6
3	C	326/327 (100%)	284 (87%)	42 (13%)	5	3
4	D	206/206 (100%)	170 (82%)	36 (18%)	2	1
5	E	168/168 (100%)	149 (89%)	19 (11%)	7	5
6	F	96/98 (98%)	86 (90%)	10 (10%)	8	6
7	G	66/71 (93%)	56 (85%)	10 (15%)	3	2
8	H	61/74 (82%)	43 (70%)	18 (30%)	0	0
9	I	44/60 (73%)	27 (61%)	17 (39%)	0	0
10	J	50/52 (96%)	41 (82%)	9 (18%)	2	1
11	K	43/46 (94%)	33 (77%)	10 (23%)	1	0
All	All	1762/1815 (97%)	1511 (86%)	251 (14%)	4	2

All (251) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	10	SER
1	A	19	LEU
1	A	32	GLN
1	A	37	VAL
1	A	50	GLU
1	A	52	ASN
1	A	58	PHE
1	A	90	SER
1	A	102	LEU
1	A	106	LEU
1	A	108	LYS
1	A	113	LEU
1	A	117	VAL
1	A	122	LEU
1	A	127	ILE
1	A	149	VAL
1	A	163	LEU
1	A	173	ASN
1	A	175	ARG
1	A	176	LYS
1	A	179	ARG
1	A	184	GLU
1	A	188	ARG
1	A	194	ARG
1	A	203	LEU
1	A	208	LEU
1	A	209	LEU
1	A	210	ASP
1	A	213	GLN
1	A	219	LEU
1	A	222	THR
1	A	226	ASP
1	A	230	THR
1	A	245	GLU
1	A	271	GLN
1	A	304	CYS
1	A	352	SER
1	A	381	ARG
1	A	388	ARG
1	A	389	ARG
1	A	392	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	430	GLN
1	A	438	ARG
1	A	445	ARG
2	B	33	LEU
2	B	35	ILE
2	B	40	ASN
2	B	46	ARG
2	B	47	ILE
2	B	69	LEU
2	B	78	LYS
2	B	97	SER
2	B	98	VAL
2	B	109	VAL
2	B	118	ILE
2	B	123	LEU
2	B	153	GLN
2	B	176	LEU
2	B	186	VAL
2	B	204	MET
2	B	211	VAL
2	B	217	LYS
2	B	227	ARG
2	B	230	LEU
2	B	232	LEU
2	B	233	SER
2	B	246	GLU
2	B	248	ASN
2	B	257	LEU
2	B	258	VAL
2	B	290	ASN
2	B	294	SER
2	B	301	LYS
2	B	305	GLN
2	B	309	VAL
2	B	315	SER
2	B	387	LEU
2	B	397	THR
2	B	421	ARG
3	C	2	THR
3	C	10	LEU
3	C	12	LYS
3	C	19	ILE

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
3	C	42	ILE
3	C	43	LEU
3	C	71	ARG
3	C	78	ILE
3	C	80	ARG
3	C	88	SER
3	C	90	PHE
3	C	92	ILE
3	C	94	LEU
3	C	102	LEU
3	C	110	LEU
3	C	114	ASN
3	C	123	VAL
3	C	164	ILE
3	C	171	ASP
3	C	177	ARG
3	C	183	PHE
3	C	241	LEU
3	C	242	LEU
3	C	243	VAL
3	C	254	ASP
3	C	255	ASN
3	C	267	HIS
3	C	269	LYS
3	C	281	LEU
3	C	287	LYS
3	C	292	LEU
3	C	294	LEU
3	C	297	SER
3	C	309	THR
3	C	320	LEU
3	C	333	LEU
3	C	336	THR
3	C	350	ILE
3	C	361	LEU
3	C	365	LEU
3	C	375	LYS
3	C	379	TRP
4	D	2	ASP
4	D	5	LEU
4	D	13	SER
4	D	24	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	D	34	LYS
4	D	35	GLN
4	D	37	CYS
4	D	40	CYS
4	D	62	LYS
4	D	66	GLU
4	D	67	GLU
4	D	68	VAL
4	D	69	GLU
4	D	76	GLU
4	D	89	ASP
4	D	93	LYS
4	D	99	GLU
4	D	106	ASN
4	D	116	ILE
4	D	136	GLU
4	D	143	LEU
4	D	167	GLU
4	D	168	VAL
4	D	170	GLU
4	D	171	PHE
4	D	179	MET
4	D	180	SER
4	D	181	GLN
4	D	184	LYS
4	D	191	ARG
4	D	203	ARG
4	D	214	LEU
4	D	223	LYS
4	D	226	LYS
4	D	234	LYS
4	D	241	LYS
5	E	12	ASP
5	E	21	SER
5	E	23	LYS
5	E	27	GLU
5	E	54	VAL
5	E	60	SER
5	E	69	LEU
5	E	71	MET
5	E	77	LYS
5	E	85	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	E	94	LYS
5	E	103	LYS
5	E	113	GLU
5	E	116	GLN
5	E	128	LYS
5	E	129	LYS
5	E	131	GLU
5	E	184	SER
5	E	188	THR
6	F	9	SER
6	F	10	SER
6	F	37	ILE
6	F	44	LYS
6	F	53	ASN
6	F	64	ARG
6	F	72	GLN
6	F	73	GLN
6	F	85	GLU
6	F	110	LYS
7	G	2	ARG
7	G	3	GLN
7	G	18	LEU
7	G	32	LYS
7	G	36	ASN
7	G	37	VAL
7	G	38	LEU
7	G	69	SER
7	G	72	LYS
7	G	73	ASN
8	H	18	THR
8	H	25	GLU
8	H	27	LEU
8	H	28	GLU
8	H	29	LYS
8	H	32	LYS
8	H	34	ARG
8	H	35	GLU
8	H	36	ARG
8	H	39	LEU
8	H	47	ARG
8	H	49	GLN
8	H	52	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
8	H	53	ASP
8	H	56	GLU
8	H	60	ASP
8	H	65	ARG
8	H	68	CYS
9	I	1	MET
9	I	7	ARG
9	I	8	SER
9	I	11	PHE
9	I	16	SER
9	I	19	SER
9	I	20	ARG
9	I	22	VAL
9	I	26	LEU
9	I	27	ARG
9	I	37	THR
9	I	38	SER
9	I	47	ARG
9	I	50	LEU
9	I	51	CYS
9	I	52	ARG
9	I	56	ARG
10	J	4	THR
10	J	18	SER
10	J	24	ILE
10	J	37	GLN
10	J	44	GLU
10	J	48	GLU
10	J	54	HIS
10	J	58	LYS
10	J	60	GLU
11	K	1	MET
11	K	2	LEU
11	K	9	ARG
11	K	13	LEU
11	K	15	ARG
11	K	18	VAL
11	K	32	LEU
11	K	39	ARG
11	K	44	TRP
11	K	53	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	GLN
1	A	141	ASN
1	A	173	ASN
1	A	274	ASN
1	A	301	ASN
1	A	305	GLN
1	A	308	GLN
1	A	323	HIS
1	A	341	GLN
1	A	359	ASN
2	B	104	ASN
2	B	143	GLN
2	B	153	GLN
2	B	162	ASN
2	B	174	ASN
2	B	276	GLN
2	B	284	HIS
2	B	313	ASN
2	B	342	ASN
2	B	343	GLN
2	B	362	ASN
2	B	385	GLN
3	C	8	HIS
3	C	32	ASN
3	C	206	ASN
3	C	322	GLN
3	C	352	GLN
6	F	53	ASN
9	I	31	GLN
11	K	12	GLN
11	K	16	ASN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 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	381	3	28,50,50	1.73	8 (28%)	17,82,82	1.04	1 (5%)
12	HEM	C	382	3	28,50,50	1.62	7 (25%)	17,82,82	1.39	2 (11%)
13	FDN	C	400	-	24,25,25	2.17	7 (29%)	24,37,37	1.74	6 (25%)
12	HEM	D	242	4	28,50,50	1.81	9 (32%)	17,82,82	1.32	2 (11%)
14	FES	E	200	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	381	3	-	0/6/54/54	0/0/8/8
12	HEM	C	382	3	-	0/6/54/54	0/0/8/8
13	FDN	C	400	-	-	0/10/29/29	0/3/3/3
12	HEM	D	242	4	-	0/6/54/54	0/0/8/8
14	FES	E	200	5	-	0/0/4/4	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	381	HEM	C3C-C2C	-3.56	1.35	1.40
13	C	400	FDN	C21-N1	-2.97	1.36	1.41
13	C	400	FDN	N1-N2	-2.94	1.34	1.40
12	D	242	HEM	C3C-C2C	-2.69	1.36	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	242	HEM	C3B-C2B	-2.53	1.37	1.40
12	C	381	HEM	C3B-C2B	-2.46	1.37	1.40
12	C	382	HEM	C3B-C2B	-2.27	1.37	1.40
12	C	382	HEM	C4D-ND	2.01	1.39	1.36
12	D	242	HEM	C1B-NB	2.02	1.39	1.36
12	C	382	HEM	C3C-CAC	2.23	1.52	1.47
12	C	381	HEM	C3C-CAC	2.27	1.52	1.47
12	C	381	HEM	CAA-C2A	2.30	1.55	1.52
12	D	242	HEM	C1C-NC	2.39	1.39	1.36
13	C	400	FDN	C12-C13	2.40	1.41	1.37
12	C	382	HEM	C1C-NC	2.45	1.39	1.36
12	D	242	HEM	CAD-C3D	2.59	1.57	1.52
13	C	400	FDN	C12-C11	2.64	1.42	1.37
12	C	381	HEM	C1B-NB	2.76	1.40	1.36
13	C	400	FDN	C9-C8	2.79	1.43	1.39
12	D	242	HEM	C3B-CAB	2.81	1.53	1.47
12	D	242	HEM	C3C-CAC	2.85	1.53	1.47
12	C	381	HEM	C1C-NC	2.86	1.40	1.36
12	C	382	HEM	C3B-CAB	2.90	1.53	1.47
13	C	400	FDN	C8-C13	3.00	1.43	1.38
12	C	381	HEM	CBB-CAB	3.44	1.53	1.28
12	C	381	HEM	CBC-CAC	3.50	1.53	1.28
12	C	382	HEM	CBC-CAC	3.61	1.54	1.28
12	C	382	HEM	CBB-CAB	3.71	1.55	1.28
12	D	242	HEM	CBB-CAB	3.81	1.55	1.28
12	D	242	HEM	CBC-CAC	3.91	1.56	1.28
13	C	400	FDN	O4-C3	5.75	1.44	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	400	FDN	C12-C13-C8	-3.04	120.67	124.07
12	C	382	HEM	CBD-CAD-C3D	-2.41	107.87	112.47
13	C	400	FDN	O6-C6-C5	-2.39	123.99	126.08
12	C	381	HEM	CBD-CAD-C3D	-2.18	108.31	112.47
13	C	400	FDN	C10-C11-C12	-2.14	120.48	123.29
12	D	242	HEM	CAA-CBA-CGA	-2.04	109.18	112.66
12	D	242	HEM	CBA-CAA-C2A	2.43	117.13	112.48
12	C	382	HEM	CAD-CBD-CGD	2.80	117.45	112.66
13	C	400	FDN	C13-C12-C11	2.94	119.86	116.65
13	C	400	FDN	F13-C13-C8	3.08	122.51	118.98
13	C	400	FDN	C21-N1-N2	4.91	125.69	116.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	381	HEM	2	0
13	C	400	FDN	1	0
12	D	242	HEM	2	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.