



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2017 – 11:22 PM EDT

PDB ID : 1P84  
Title : HDBT inhibited Yeast Cytochrome bc1 Complex  
Authors : Palsdottir, H.; Lojero, C.G.; Trumpower, B.L.; Hunte, C.  
Deposited on : unknown  
Resolution : 2.50 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.

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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 : 1.7.2 (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) : rb-20030345

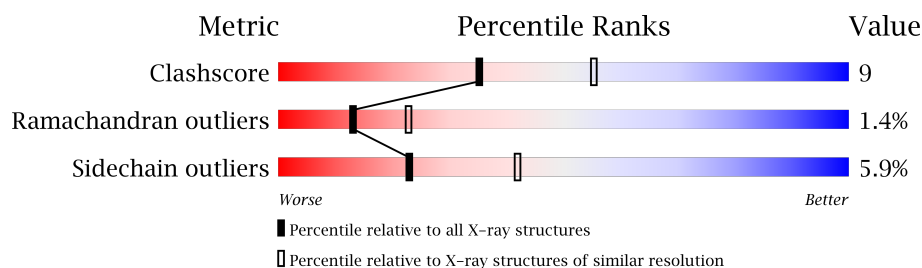
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)

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	431	<div> <div>76%</div> <div>22%</div> <div>.</div> </div>
2	B	352	<div> <div>63%</div> <div>35%</div> <div>.</div> </div>
3	C	385	<div> <div>85%</div> <div>14%</div> <div>.</div> </div>
4	D	246	<div> <div>83%</div> <div>15%</div> <div>.</div> </div>
5	E	185	<div> <div>82%</div> <div>17%</div> <div>.</div> </div>
6	F	74	<div> <div>78%</div> <div>20%</div> <div>.</div> </div>
7	G	125	<div> <div>90%</div> <div>10%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
8	H	93	<div><div></div><div>85%</div><div>13%</div><div></div></div>
9	I	55	<div><div></div><div>85%</div><div>11%</div><div></div></div>
10	J	127	<div><div></div><div>69%</div><div>26%</div><div>5%</div></div>
11	K	107	<div><div></div><div>60%</div><div>35%</div><div>6%</div></div>

## 2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 18069 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3344	2109	576	653	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ASP	GLU	CONFLICT	UNP P07256

- Molecule 2 is a protein called Ubiquinol-cytochrome C reductase complex core protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	352	Total	C	N	O	S	0	0	0
			2735	1747	453	534	1			

- Molecule 3 is a protein called cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	385	Total	C	N	O	S	0	0	0
			3089	2080	484	504	21			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	122	THR	ILE	CONFLICT	UNP P00163

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	246	Total	C	N	O	S	0	0	0
			1941	1237	334	361	9			

- Molecule 5 is a protein called Ubiquinol-cytochrome C reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	185	Total	C	N	O	S	0	0	0
			1411	893	242	266	10			

- Molecule 6 is a protein called Ubiquinol-cytochrome C reductase complex 17 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	74	Total	C	N	O	S	0	0	0
			624	391	108	123	2			

- Molecule 7 is a protein called Ubiquinol-cytochrome C reductase complex 14 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	125	Total	C	N	O	S	0	0	0
			1012	648	172	190	2			

- Molecule 8 is a protein called Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	93	Total	C	N	O	S	98	0	0
			773	510	131	130	2			

- Molecule 9 is a protein called Ubiquinol-cytochrome C reductase complex 7.3 kDa protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	55	Total	C	N	O	0	0	0
			449	298	75	76			

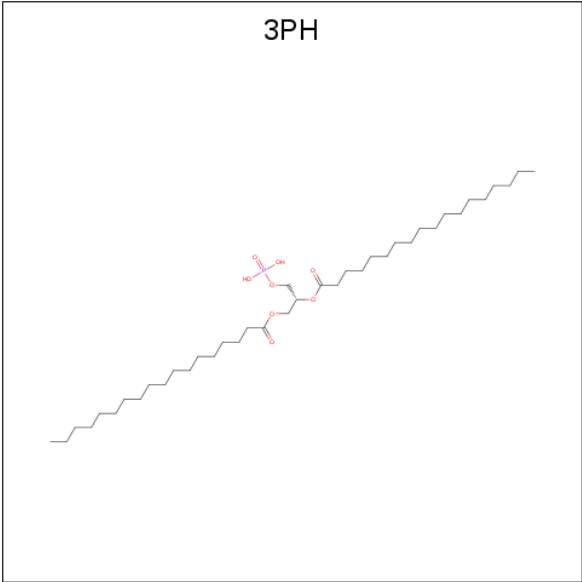
- Molecule 10 is a protein called Heavy Chain (Vh) Of Fv-Fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	127	Total	C	N	O	S	0	0	0
			1015	644	167	201	3			

- Molecule 11 is a protein called Light Chain (Vl) Of Fv-Fragment.

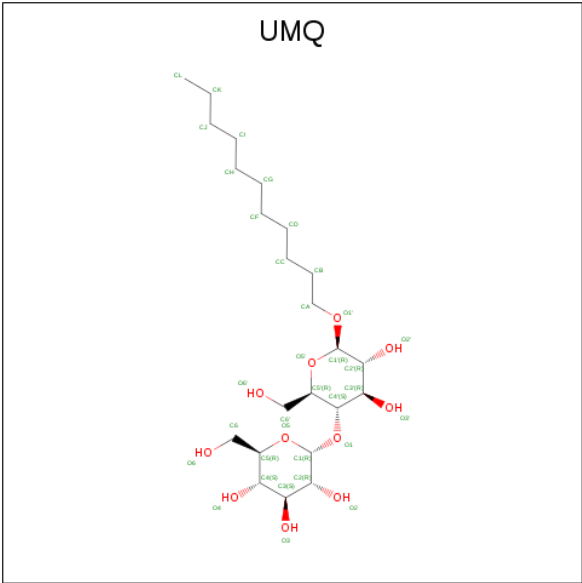
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	107	Total	C	N	O	S	0	0	0
			842	536	141	163	2			

- Molecule 12 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: C<sub>39</sub>H<sub>77</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	O	P	0	0
			40	31	8	1		
12	D	1	Total	C	O	P	0	0
			38	29	8	1		

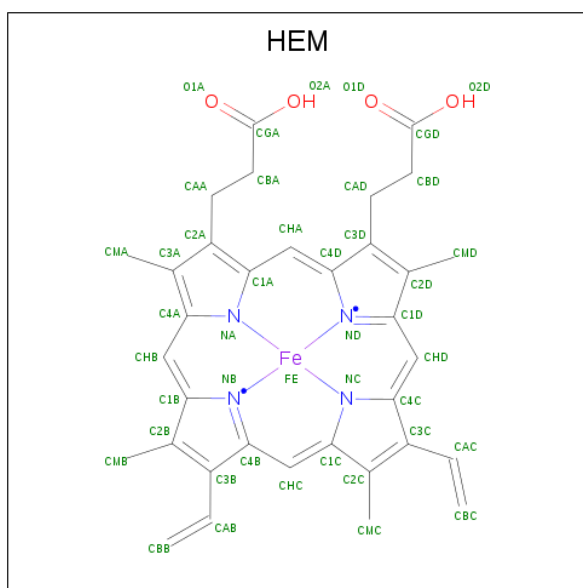
- Molecule 13 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: C<sub>23</sub>H<sub>44</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	O	0	0
			34	23	11		

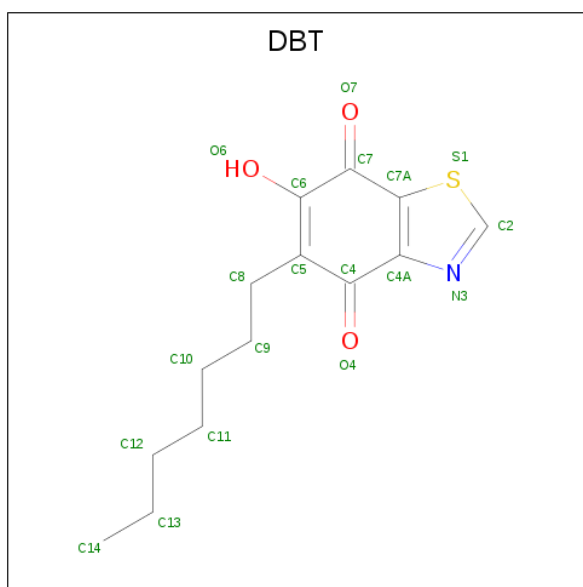
- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula:  $C_{34}H_{32}FeN_4O_4$ ).



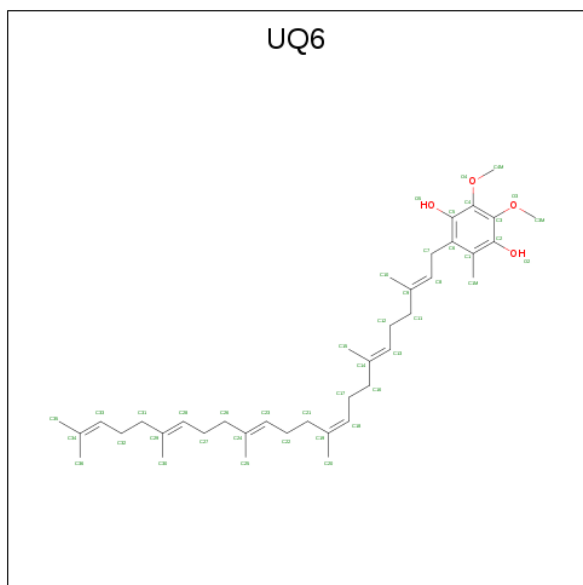
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
14	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
14	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 15 is 5-HEPTYL-6-HYDROXY-1,3-BENZOTHAZOLE-4,7-DIONE (three-letter code: DBT) (formula:  $C_{14}H_{17}NO_3S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	N	O	S	0	0
			19	14	1	3	1		

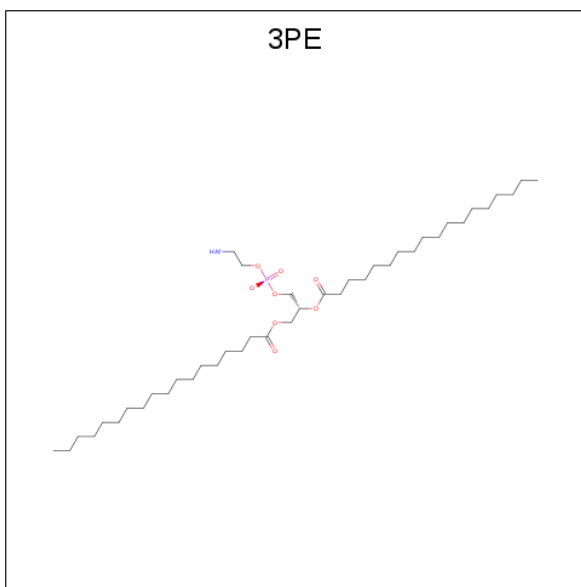
- Molecule 16 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXAENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (three-letter code: UQ6) (formula:  $C_{39}H_{60}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O	0	0
			43	39	4		

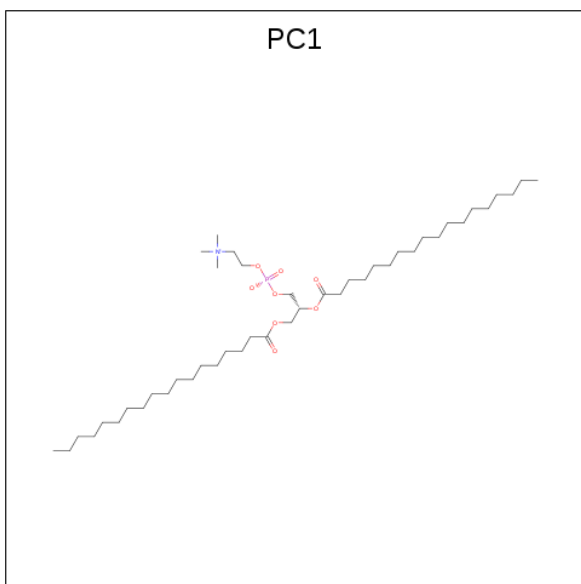
- Molecule 17 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).





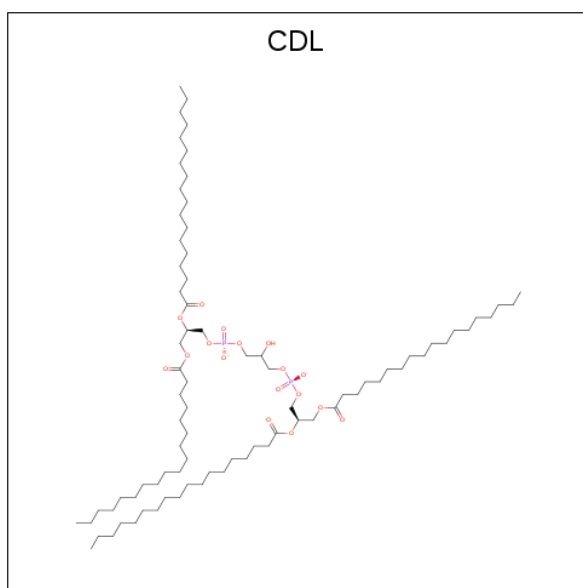
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	C	1	Total	C	N	O	P	0	0
			47	37	1	8	1		
17	C	1	Total	C	N	O	P	0	0
			40	30	1	8	1		

- Molecule 18 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula:  $C_{44}H_{88}NO_8P$ ).



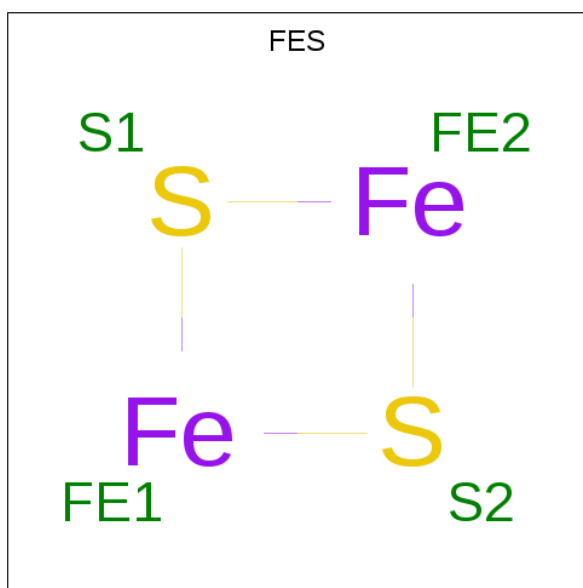
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	D	1	Total	C	N	O	P	0	0
			38	28	1	8	1		

- Molecule 19 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	D	1	Total	C	O	P	0	0
			76	57	17	2		

- Molecule 20 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $Fe_2S_2$ ).



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

- Molecule 21 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	55	Total O 55 55	0	0
21	B	11	Total O 11 11	0	0
21	C	110	Total O 110 110	0	0
21	D	62	Total O 62 62	0	0
21	E	25	Total O 25 25	0	0
21	F	4	Total O 4 4	0	0
21	G	32	Total O 32 32	0	0
21	H	20	Total O 20 20	0	0
21	I	2	Total O 2 2	0	0
21	J	3	Total O 3 3	0	0
21	K	2	Total O 2 2	0	0

### 3 Residue-property plots

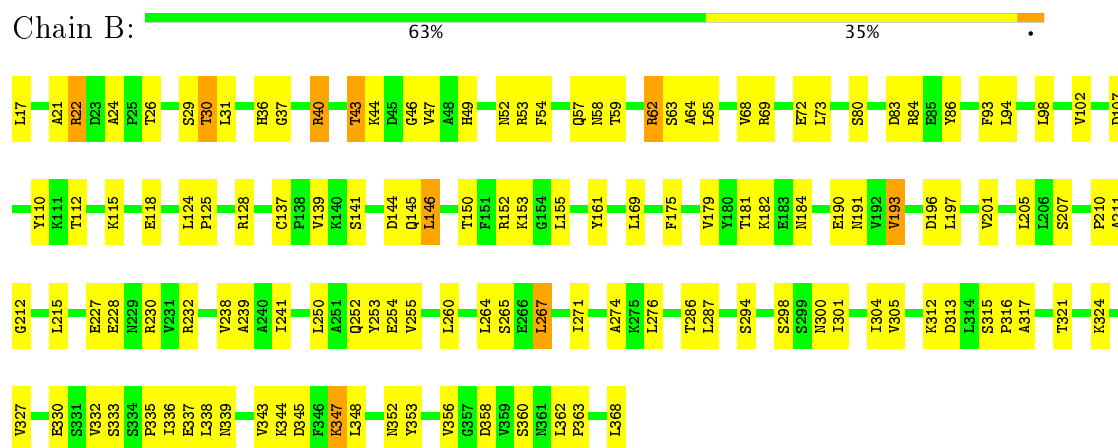
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

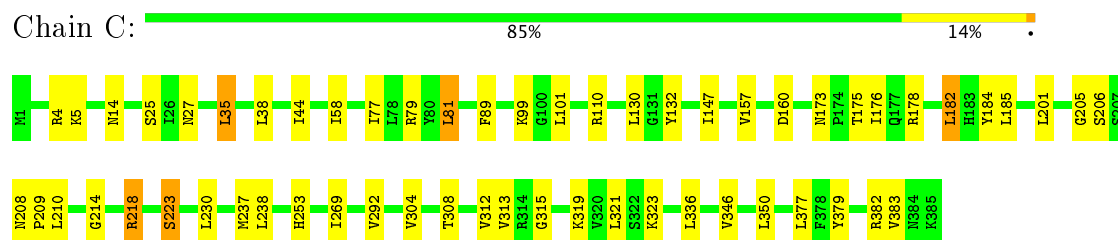
- Molecule 1: Ubiquinol-cytochrome C reductase complex core protein I



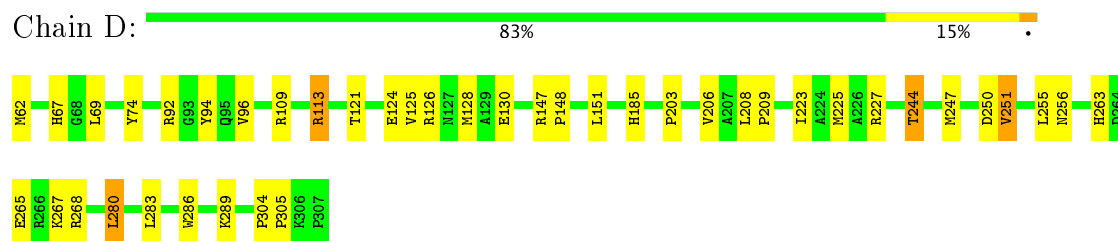
- Molecule 2: Ubiquinol-cytochrome C reductase complex core protein 2



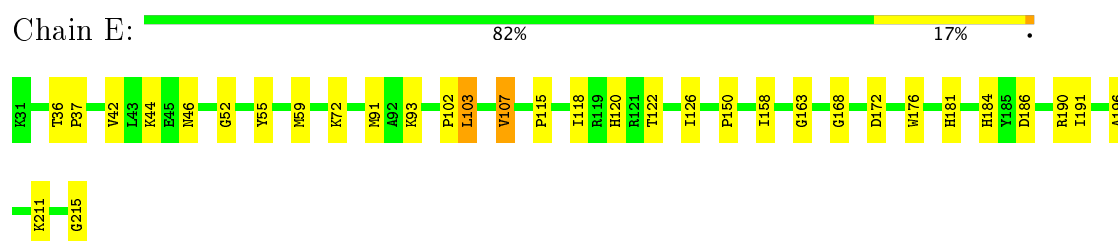
- Molecule 3: cytochrome b



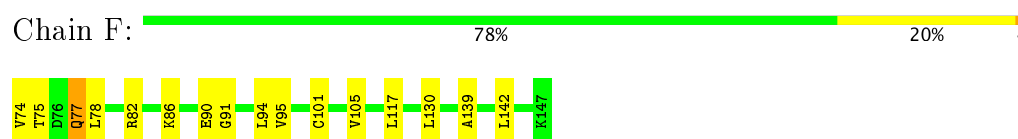
- Molecule 4: Cytochrome c1, heme protein



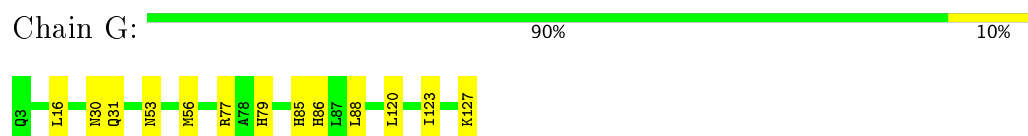
- Molecule 5: Ubiquinol-cytochrome C reductase iron-sulfur subunit



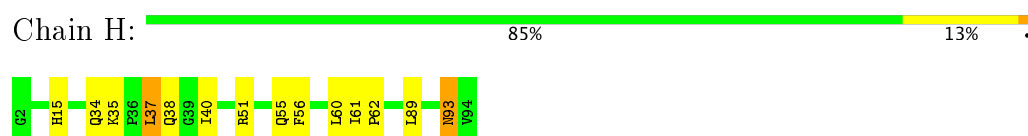
- Molecule 6: Ubiquinol-cytochrome C reductase complex 17 kDa protein



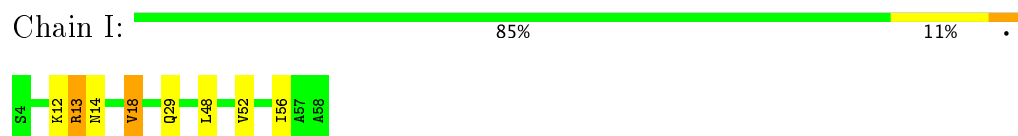
- Molecule 7: Ubiquinol-cytochrome C reductase complex 14 kDa protein



- Molecule 8: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C

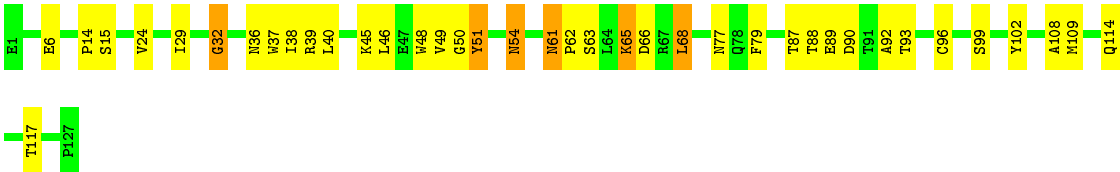


- Molecule 9: Ubiquinol-cytochrome C reductase complex 7.3 kDa protein

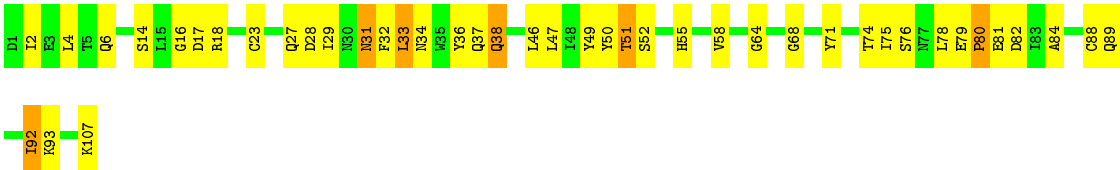


- Molecule 10: Heavy Chain (Vh) Of Fv-Fragment





• Molecule 11: Light Chain (VI) Of Fv-Fragment



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	215.00Å 165.09Å 147.53Å 90.00° 117.33° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50	Depositor
% Data completeness (in resolution range)	92.5 (25.00-2.50)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.228 , 0.252	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18069	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	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: UMQ, CDL, PC1, 3PE, 3PH, FES, HEM, DBT, UQ6

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	0.36	0/3405	0.59	0/4614
2	B	0.33	0/2781	0.59	0/3764
3	C	0.45	0/3191	0.64	1/4353 (0.0%)
4	D	0.37	0/2002	0.60	0/2726
5	E	0.35	0/1444	0.61	1/1957 (0.1%)
6	F	0.34	0/638	0.54	0/858
7	G	0.37	0/1032	0.64	0/1397
8	H	0.40	0/804	0.52	0/1088
9	I	0.41	0/462	0.50	0/622
10	J	0.35	0/1043	0.64	1/1422 (0.1%)
11	K	0.33	0/863	0.57	0/1172
All	All	0.37	0/17665	0.60	3/23973 (0.0%)

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
4	D	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	32	GLY	N-CA-C	6.55	129.48	113.10
3	C	346	VAL	N-CA-C	5.96	127.08	111.00
5	E	163	GLY	N-CA-C	5.45	126.73	113.10

There are no chirality outliers.



All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	94	TYR	Sidechain

## 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	3344	0	3321	70	0
2	B	2735	0	2774	83	0
3	C	3089	0	3125	33	0
4	D	1941	0	1862	25	0
5	E	1411	0	1386	24	0
6	F	624	0	581	11	0
7	G	1012	0	1026	9	0
8	H	773	0	736	12	0
9	I	449	0	445	6	0
10	J	1015	0	959	30	0
11	K	842	0	820	25	0
12	A	40	0	53	4	0
12	D	38	0	49	3	0
13	A	34	0	44	2	0
14	C	86	0	60	1	0
14	D	43	0	30	0	0
15	C	19	0	17	1	0
16	C	43	0	58	8	0
17	C	87	0	128	3	0
18	D	38	0	50	3	0
19	D	76	0	99	5	0
20	E	4	0	0	1	0
21	A	55	0	0	1	0
21	B	11	0	0	0	0
21	C	110	0	0	5	0
21	D	62	0	0	0	0
21	E	25	0	0	0	0
21	F	4	0	0	1	0
21	G	32	0	0	1	0
21	H	20	0	0	1	0
21	I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	J	3	0	0	0	0
21	K	2	0	0	0	0
All	All	18069	0	17623	328	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 9.

All (328) 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)
16:C:706:UQ6:H1M1	16:C:706:UQ6:H103	1.31	1.10
6:F:77:GLN:H	6:F:77:GLN:HE21	1.01	0.98
17:C:710:3PE:H111	8:H:51:ARG:HD2	1.53	0.90
2:B:182:LYS:HB2	2:B:211:ALA:HB2	1.58	0.86
6:F:77:GLN:H	6:F:77:GLN:NE2	1.75	0.85
1:A:63:ASN:HB2	1:A:66:ASN:ND2	1.91	0.84
1:A:317:HIS:HE1	1:A:351:TRP:HE1	1.25	0.83
2:B:347:LYS:HD3	2:B:347:LYS:H	1.43	0.81
16:C:706:UQ6:C10	16:C:706:UQ6:H1M1	2.11	0.80
2:B:49:HIS:HD2	2:B:161:TYR:H	1.28	0.80
2:B:336:ILE:HG21	2:B:339:ASN:HB2	1.63	0.80
16:C:706:UQ6:C1M	16:C:706:UQ6:H103	2.10	0.79
2:B:300:ASN:O	2:B:304:ILE:HG12	1.84	0.77
2:B:146:LEU:HD23	2:B:286:THR:HG22	1.68	0.76
3:C:58:ILE:H	3:C:173:ASN:HD22	1.34	0.76
12:A:713:3PH:H12	21:A:775:HOH:O	1.85	0.75
2:B:305:VAL:HG21	2:B:368:LEU:HD22	1.69	0.74
19:D:731:CDL:HB22	7:G:85:HIS:NE2	2.03	0.74
19:D:731:CDL:H351	19:D:731:CDL:H151	1.69	0.74
6:F:77:GLN:HE21	6:F:77:GLN:N	1.83	0.72
11:K:32:PHE:HD2	11:K:92:ILE:HG22	1.54	0.72
2:B:30:THR:HG23	2:B:190:GLU:HB3	1.69	0.72
3:C:147:ILE:HD11	15:C:705:DBT:H92	1.72	0.72
2:B:336:ILE:HD12	2:B:336:ILE:H	1.55	0.71
2:B:49:HIS:CD2	2:B:161:TYR:H	2.07	0.70
2:B:254:GLU:HG2	2:B:276:LEU:HD23	1.74	0.70
3:C:176:ILE:N	21:C:809:HOH:O	2.25	0.69
1:A:73:TRP:CE3	1:A:76:ILE:HD11	2.27	0.69
1:A:63:ASN:HB2	1:A:66:ASN:HD21	1.56	0.68
2:B:336:ILE:CG2	2:B:339:ASN:HB2	2.23	0.68
7:G:77:ARG:HD3	7:G:88:LEU:HD11	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLY:H	1:A:61:ASN:ND2	1.92	0.67
6:F:78:LEU:HD13	6:F:142:LEU:HD22	1.74	0.67
1:A:99:ARG:HD3	1:A:174:LEU:HD12	1.74	0.67
3:C:27:ASN:HB2	19:D:731:CDL:OB3	1.95	0.67
3:C:58:ILE:H	3:C:173:ASN:ND2	1.91	0.67
3:C:208:ASN:HD22	3:C:210:LEU:H	1.40	0.67
1:A:289:ASN:HD22	1:A:289:ASN:C	2.00	0.65
10:J:29:ILE:H	10:J:77:ASN:HD21	1.42	0.65
1:A:42:HIS:CD2	1:A:42:HIS:H	2.15	0.65
5:E:107:VAL:HG12	5:E:118:ILE:HB	1.77	0.64
6:F:91:GLY:O	6:F:95:VAL:HG13	1.98	0.64
6:F:74:VAL:HG12	6:F:75:THR:H	1.62	0.64
1:A:109:LEU:HG	1:A:110:PRO:HD2	1.80	0.64
2:B:40:ARG:HG3	2:B:155:LEU:HG	1.80	0.63
2:B:65:LEU:O	2:B:69:ARG:HG2	1.99	0.63
12:A:713:3PH:H282	3:C:230:LEU:HD13	1.81	0.63
2:B:110:TYR:HD2	2:B:205:LEU:HD23	1.64	0.62
11:K:37:GLN:HB2	11:K:47:LEU:HD11	1.81	0.62
3:C:132:TYR:OH	3:C:253:HIS:HD2	1.83	0.61
11:K:27:GLN:HG2	11:K:28:ASP:H	1.65	0.61
6:F:82:ARG:O	6:F:86:LYS:HG3	2.00	0.61
1:A:172:THR:HG23	1:A:173:PRO:HD2	1.83	0.61
11:K:29:ILE:HG22	11:K:92:ILE:HD12	1.81	0.61
5:E:115:PRO:HD2	5:E:158:ILE:HD11	1.83	0.61
11:K:2:ILE:H	11:K:2:ILE:HD12	1.65	0.61
2:B:264:LEU:HD12	2:B:317:ALA:HB2	1.82	0.61
4:D:113:ARG:HG2	4:D:151:LEU:O	2.00	0.61
11:K:29:ILE:HA	11:K:92:ILE:HG21	1.82	0.61
11:K:47:LEU:HA	11:K:58:VAL:HG11	1.84	0.60
10:J:61:ASN:HD22	10:J:63:SER:H	1.48	0.60
2:B:181:THR:HB	2:B:212:GLY:H	1.66	0.60
2:B:305:VAL:HG11	2:B:368:LEU:HB3	1.84	0.59
1:A:289:ASN:ND2	1:A:291:PHE:H	2.01	0.59
1:A:46:ALA:O	1:A:47:HIS:HB2	2.03	0.58
2:B:24:ALA:HB3	2:B:191:ASN:ND2	2.18	0.58
1:A:229:SER:HB3	1:A:232:THR:HB	1.85	0.58
10:J:6:GLU:H	10:J:114:GLN:HE21	1.49	0.58
3:C:4:ARG:HE	3:C:14:ASN:ND2	2.01	0.58
2:B:182:LYS:HD3	2:B:207:SER:HA	1.86	0.58
5:E:103:LEU:O	5:E:120:HIS:HB3	2.04	0.58
5:E:44:LYS:NZ	5:E:52:GLY:H	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:77:ARG:HD2	21:G:149:HOH:O	2.04	0.58
2:B:287:LEU:HD21	2:B:304:ILE:HG21	1.85	0.58
1:A:252:ARG:HD3	1:A:254:ASP:OD1	2.04	0.57
1:A:313:ASP:OD1	1:A:335:ARG:HD3	2.05	0.57
4:D:185:HIS:ND1	18:D:715:PC1:H142	2.19	0.57
1:A:258:LYS:HG2	1:A:335:ARG:HG3	1.87	0.57
10:J:99:SER:HB3	10:J:109:MET:HG2	1.87	0.56
10:J:61:ASN:ND2	10:J:63:SER:H	2.03	0.56
1:A:289:ASN:HD22	1:A:291:PHE:H	1.51	0.56
5:E:44:LYS:HB3	8:H:35:LYS:HA	1.87	0.56
11:K:38:GLN:O	11:K:84:ALA:HB1	2.05	0.56
5:E:191:ILE:HD13	5:E:196:ALA:HB3	1.88	0.56
10:J:36:ASN:OD1	10:J:51:TYR:HB3	2.05	0.56
1:A:306:ILE:HA	1:A:311:LEU:HD22	1.87	0.56
8:H:89:LEU:O	8:H:93:ASN:HB2	2.05	0.55
10:J:6:GLU:H	10:J:114:GLN:NE2	2.04	0.55
1:A:74:LYS:HG3	1:A:95:SER:HB3	1.88	0.55
3:C:214:GLY:O	3:C:218:ARG:HD2	2.06	0.55
1:A:73:TRP:CZ3	1:A:76:ILE:HD11	2.41	0.55
3:C:315:GLY:HA3	21:C:814:HOH:O	2.06	0.55
5:E:172:ASP:H	5:E:184:HIS:HD2	1.54	0.55
1:A:67:ASN:ND2	1:A:180:GLY:HA2	2.21	0.55
2:B:98:LEU:O	2:B:102:VAL:HG23	2.06	0.55
10:J:38:ILE:HA	10:J:49:VAL:HG23	1.89	0.55
3:C:323:LYS:CE	8:H:55:GLN:HE22	2.20	0.54
3:C:44:ILE:HD12	16:C:706:UQ6:C20	2.37	0.54
3:C:4:ARG:HE	3:C:14:ASN:HD21	1.55	0.54
11:K:34:ASN:HD22	11:K:49:TYR:HA	1.73	0.54
17:C:710:3PE:C11	8:H:51:ARG:HD2	2.33	0.54
9:I:52:VAL:O	9:I:56:ILE:HG12	2.07	0.54
2:B:36:HIS:HB2	2:B:184:ASN:OD1	2.08	0.53
3:C:173:ASN:O	21:C:809:HOH:O	2.19	0.53
5:E:55:TYR:O	5:E:59:MET:HG2	2.08	0.53
1:A:58:GLY:H	1:A:61:ASN:HD22	1.55	0.53
12:D:714:3PH:H2A2	12:D:714:3PH:H251	1.89	0.53
2:B:252:GLN:HG3	2:B:253:TYR:N	2.22	0.53
2:B:93:PHE:HD1	2:B:94:LEU:O	1.91	0.53
10:J:87:THR:HG22	10:J:88:THR:N	2.23	0.53
2:B:313:ASP:O	2:B:316:PRO:HD3	2.08	0.53
1:A:350:GLN:HE22	1:A:353:ARG:HH21	1.57	0.53
11:K:31:ASN:ND2	11:K:51:THR:HG21	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:208:ASN:HB2	3:C:209:PRO:HD2	1.91	0.53
3:C:25:SER:OG	7:G:79:HIS:HD2	1.92	0.52
2:B:110:TYR:CD2	2:B:205:LEU:HD23	2.44	0.52
4:D:247:MET:O	4:D:251:VAL:HG22	2.09	0.52
7:G:31:GLN:HA	7:G:31:GLN:NE2	2.24	0.52
5:E:93:LYS:HD3	5:E:215:GLY:HA3	1.91	0.52
1:A:68:GLY:HA3	1:A:185:LEU:HD11	1.92	0.52
1:A:217:GLU:HA	1:A:220:VAL:HG12	1.91	0.52
1:A:169:PHE:O	1:A:172:THR:HB	2.09	0.52
3:C:208:ASN:ND2	3:C:210:LEU:H	2.08	0.52
8:H:61:ILE:HB	8:H:62:PRO:HD3	1.92	0.52
1:A:77:PHE:CE1	1:A:124:PHE:HE1	2.28	0.51
1:A:265:VAL:HG21	1:A:426:LEU:HD12	1.93	0.51
1:A:172:THR:HG23	1:A:242:ALA:HA	1.91	0.51
3:C:77:ILE:O	3:C:81:LEU:HB2	2.11	0.51
2:B:315:SER:N	2:B:316:PRO:HD3	2.25	0.51
4:D:286:TRP:CE3	5:E:59:MET:HG3	2.45	0.51
1:A:156:HIS:HD2	1:A:159:ARG:HH21	1.57	0.51
2:B:115:LYS:HB2	2:B:118:GLU:HG3	1.92	0.51
1:A:172:THR:CG2	1:A:242:ALA:HA	2.40	0.51
4:D:147:ARG:HG2	4:D:148:PRO:O	2.10	0.51
5:E:103:LEU:HA	5:E:120:HIS:ND1	2.26	0.51
2:B:83:ASP:HB2	2:B:86:TYR:H	1.75	0.50
1:A:235:LYS:HB2	1:A:235:LYS:NZ	2.26	0.50
1:A:373:GLN:HG3	1:A:374:LEU:N	2.26	0.50
4:D:96:VAL:HB	4:D:251:VAL:HG13	1.94	0.50
4:D:263:HIS:NE2	4:D:267:LYS:HE3	2.26	0.50
11:K:4:LEU:HD23	11:K:88:CYS:SG	2.51	0.50
2:B:347:LYS:HG2	2:B:348:LEU:N	2.27	0.50
2:B:52:ASN:HD21	2:B:80:SER:C	2.15	0.50
3:C:175:THR:O	3:C:178:ARG:HG2	2.12	0.50
11:K:36:TYR:HE2	11:K:89:GLN:HG2	1.76	0.50
4:D:203:PRO:HG2	4:D:206:VAL:HG21	1.94	0.50
2:B:46:GLY:O	2:B:49:HIS:HB3	2.12	0.49
2:B:324:LYS:O	2:B:327:VAL:HG22	2.12	0.49
4:D:62:MET:HB3	4:D:67:HIS:NE2	2.27	0.49
6:F:101:CYS:O	6:F:105:VAL:HG23	2.13	0.49
6:F:90:GLU:HB3	21:F:149:HOH:O	2.12	0.49
10:J:37:TRP:CZ3	10:J:96:CYS:HB3	2.47	0.49
10:J:48:TRP:CZ2	10:J:50:GLY:HA2	2.48	0.49
2:B:182:LYS:HB2	2:B:211:ALA:CB	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:267:LEU:HD22	2:B:304:ILE:HD13	1.94	0.49
7:G:31:GLN:HA	7:G:31:GLN:HE21	1.77	0.49
10:J:99:SER:HA	10:J:108:ALA:O	2.13	0.48
11:K:6:GLN:HG2	11:K:23:CYS:SG	2.53	0.48
2:B:298:SER:OG	2:B:363:PRO:HD3	2.13	0.48
2:B:347:LYS:N	2:B:347:LYS:HD3	2.19	0.48
10:J:61:ASN:HD22	10:J:62:PRO:N	2.11	0.48
2:B:62:ARG:HH21	2:B:62:ARG:HB2	1.77	0.48
13:A:721:UMQ:O2'	9:I:18:VAL:HG22	2.14	0.48
2:B:197:LEU:O	2:B:201:VAL:HG23	2.13	0.48
2:B:26:THR:OG1	2:B:191:ASN:ND2	2.47	0.48
6:F:74:VAL:HG12	6:F:75:THR:N	2.28	0.48
1:A:127:GLN:C	1:A:129:ALA:H	2.17	0.48
4:D:125:VAL:HA	4:D:128:MET:HE3	1.96	0.48
5:E:168:GLY:HA2	5:E:176:TRP:CD1	2.48	0.48
2:B:58:ASN:OD1	2:B:63:SER:HA	2.14	0.48
5:E:172:ASP:H	5:E:184:HIS:CD2	2.31	0.48
1:A:179:ARG:HG2	1:A:179:ARG:HH21	1.78	0.47
5:E:181:HIS:HB2	20:E:704:FES:S1	2.54	0.47
10:J:54:ASN:H	10:J:54:ASN:HD22	1.62	0.47
1:A:67:ASN:HD22	1:A:181:THR:HG23	1.79	0.47
2:B:241:ILE:HA	2:B:352:ASN:O	2.15	0.47
2:B:52:ASN:ND2	2:B:80:SER:OG	2.47	0.47
1:A:77:PHE:HE1	1:A:124:PHE:HE1	1.60	0.47
1:A:117:LEU:HD11	1:A:219:LEU:HD12	1.96	0.47
3:C:379:TYR:CE1	3:C:383:VAL:HG21	2.50	0.47
1:A:349:LYS:HA	1:A:349:LYS:HD3	1.63	0.47
4:D:286:TRP:CD2	8:H:37:LEU:HD12	2.50	0.47
1:A:288:TYR:HB3	1:A:315:PHE:CE2	2.50	0.47
2:B:124:LEU:HB2	2:B:125:PRO:HD3	1.96	0.47
10:J:93:THR:HG22	10:J:117:THR:HG23	1.97	0.47
11:K:74:THR:HG22	11:K:75:ILE:N	2.29	0.47
11:K:52:SER:HB3	11:K:64:GLY:O	2.15	0.47
1:A:456:ARG:HH21	1:A:456:ARG:HG3	1.80	0.47
2:B:21:ALA:O	2:B:22:ARG:HB2	2.14	0.47
2:B:59:THR:HA	2:B:112:THR:HA	1.97	0.47
1:A:68:GLY:HA3	1:A:185:LEU:CD1	2.45	0.46
10:J:40:LEU:O	10:J:92:ALA:HB1	2.15	0.46
12:A:713:3PH:H3B2	12:D:714:3PH:H382	1.97	0.46
5:E:72:LYS:NZ	9:I:29:GLN:NE2	2.63	0.46
2:B:274:ALA:HB2	2:B:287:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:121:THR:OG1	4:D:124:GLU:HG3	2.15	0.46
11:K:2:ILE:HD12	11:K:2:ILE:N	2.29	0.46
11:K:14:SER:HB2	11:K:17:ASP:OD2	2.16	0.46
3:C:313:VAL:HG22	3:C:319:LYS:HE3	1.98	0.46
1:A:350:GLN:NE2	1:A:353:ARG:HD3	2.30	0.46
1:A:58:GLY:N	1:A:61:ASN:ND2	2.62	0.46
1:A:63:ASN:HB2	1:A:66:ASN:HD22	1.75	0.46
1:A:86:ALA:HB2	1:A:119:PHE:CZ	2.51	0.46
2:B:252:GLN:O	2:B:255:VAL:HG22	2.16	0.46
5:E:122:THR:O	5:E:126:ILE:HG13	2.17	0.46
1:A:86:ALA:HB2	1:A:119:PHE:CE1	2.51	0.45
1:A:67:ASN:ND2	1:A:181:THR:HG23	2.31	0.45
10:J:45:LYS:O	10:J:45:LYS:HG3	2.16	0.45
11:K:46:LEU:HD23	11:K:55:HIS:CD2	2.51	0.45
11:K:32:PHE:CD2	11:K:92:ILE:HG22	2.43	0.45
3:C:201:LEU:HD21	16:C:706:UQ6:H3M2	1.98	0.45
2:B:44:LYS:HB2	2:B:47:VAL:HG21	1.97	0.45
8:H:56:PHE:O	8:H:60:LEU:HB2	2.17	0.45
10:J:61:ASN:HD22	10:J:61:ASN:C	2.19	0.45
3:C:35:LEU:HD13	21:C:727:HOH:O	2.16	0.45
5:E:150:PRO:HB3	10:J:102:TYR:CE2	2.52	0.45
1:A:49:ALA:HA	1:A:212:GLY:HA3	1.98	0.45
2:B:313:ASP:HB3	2:B:344:LYS:O	2.16	0.45
11:K:50:TYR:O	11:K:51:THR:HG22	2.16	0.45
3:C:173:ASN:C	21:C:809:HOH:O	2.53	0.45
1:A:429:GLN:HE22	9:I:13:ARG:NH2	2.15	0.45
7:G:120:LEU:O	7:G:123:ILE:HG12	2.17	0.45
2:B:252:GLN:HB3	2:B:343:VAL:HG21	1.99	0.45
7:G:53:ASN:ND2	7:G:56:MET:H	2.15	0.45
2:B:69:ARG:O	2:B:73:LEU:HD23	2.17	0.44
19:D:731:CDL:HB22	7:G:85:HIS:HE2	1.82	0.44
10:J:14:PRO:O	10:J:15:SER:HB3	2.17	0.44
10:J:29:ILE:HG12	10:J:77:ASN:ND2	2.32	0.44
8:H:15:HIS:HB3	21:H:106:HOH:O	2.16	0.44
2:B:228:GLU:HA	2:B:353:TYR:O	2.17	0.44
10:J:49:VAL:CG1	10:J:68:LEU:HD23	2.47	0.44
1:A:317:HIS:HE1	1:A:351:TRP:NE1	2.05	0.44
1:A:121:ASN:ND2	1:A:125:ILE:HD12	2.33	0.44
5:E:191:ILE:CD1	5:E:196:ALA:HB3	2.47	0.44
2:B:29:SER:HA	2:B:191:ASN:HB3	2.00	0.44
1:A:142:LYS:NZ	1:A:142:LYS:HB2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:LEU:HD12	2:B:155:LEU:H	1.82	0.44
2:B:155:LEU:HD12	2:B:155:LEU:N	2.32	0.44
4:D:203:PRO:HG2	4:D:206:VAL:CG2	2.48	0.44
1:A:289:ASN:ND2	1:A:289:ASN:C	2.70	0.44
1:A:29:VAL:HG11	1:A:400:LYS:HB3	1.99	0.44
1:A:58:GLY:N	1:A:61:ASN:HD22	2.15	0.44
14:C:702:HEM:HMC2	14:C:702:HEM:HBC2	2.00	0.44
4:D:304:PRO:HA	4:D:305:PRO:HD3	1.84	0.44
1:A:350:GLN:NE2	1:A:353:ARG:HH21	2.16	0.44
1:A:430:ASP:OD2	1:A:449:ARG:NH2	2.50	0.44
4:D:74:TYR:CE1	6:F:139:ALA:HA	2.53	0.44
2:B:141:SER:O	2:B:145:GLN:HG2	2.17	0.43
5:E:186:ASP:OD2	5:E:190:ARG:HD2	2.18	0.43
11:K:33:LEU:HD22	11:K:71:TYR:CG	2.53	0.43
1:A:69:VAL:HG13	1:A:70:SER:N	2.33	0.43
2:B:40:ARG:HB2	2:B:84:ARG:O	2.19	0.43
5:E:42:VAL:HG12	8:H:34:GLN:HG2	1.99	0.43
2:B:239:ALA:HB1	2:B:301:ILE:HD12	2.00	0.43
18:D:715:PC1:H153	18:D:715:PC1:O12	2.18	0.43
10:J:87:THR:HG22	10:J:88:THR:H	1.83	0.43
2:B:294:SER:HB3	2:B:358:ASP:HB3	2.01	0.43
10:J:38:ILE:O	10:J:38:ILE:HG13	2.19	0.43
12:A:713:3PH:H282	3:C:230:LEU:CD1	2.48	0.43
2:B:43:THR:HG22	2:B:175:PHE:HD1	1.82	0.43
1:A:179:ARG:H	1:A:179:ARG:HD2	1.83	0.43
2:B:193:VAL:HG23	2:B:196:ASP:HB2	2.01	0.43
3:C:110:ARG:NH2	3:C:205:GLY:O	2.52	0.43
5:E:72:LYS:HZ2	9:I:29:GLN:NE2	2.16	0.43
1:A:66:ASN:H	1:A:66:ASN:HD22	1.67	0.43
10:J:24:VAL:HG21	10:J:29:ILE:HD11	2.01	0.42
10:J:65:LYS:HA	10:J:68:LEU:HD11	2.00	0.42
2:B:250:LEU:HD21	2:B:336:ILE:HD13	2.01	0.42
4:D:255:LEU:HD23	4:D:255:LEU:HA	1.88	0.42
11:K:79:GLU:HA	11:K:80:PRO:HA	1.87	0.42
2:B:175:PHE:CE2	2:B:179:VAL:HG21	2.55	0.42
2:B:232:ARG:HH21	2:B:232:ARG:HB3	1.84	0.42
5:E:36:THR:HA	5:E:37:PRO:HD2	1.92	0.42
10:J:29:ILE:H	10:J:77:ASN:ND2	2.15	0.42
2:B:260:LEU:O	2:B:271:ILE:HD11	2.20	0.42
3:C:304:VAL:HG13	3:C:308:THR:HG23	2.02	0.42
1:A:172:THR:HG21	1:A:243:ALA:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:ARG:HH21	2:B:62:ARG:CB	2.33	0.42
2:B:64:ALA:O	2:B:68:VAL:HG23	2.19	0.42
11:K:4:LEU:CD2	11:K:88:CYS:SG	3.08	0.42
11:K:75:ILE:HG22	11:K:76:SER:N	2.35	0.42
2:B:150:THR:HG22	2:B:352:ASN:ND2	2.35	0.42
10:J:38:ILE:HD12	10:J:46:LEU:HD22	2.02	0.42
1:A:313:ASP:OD2	1:A:335:ARG:NH2	2.53	0.41
10:J:51:TYR:CD2	10:J:51:TYR:C	2.94	0.41
1:A:317:HIS:CE1	1:A:351:TRP:HE1	2.17	0.41
2:B:145:GLN:HA	2:B:145:GLN:NE2	2.36	0.41
3:C:157:VAL:O	3:C:160:ASP:HB2	2.20	0.41
4:D:265:GLU:OE2	4:D:268:ARG:NH2	2.53	0.41
2:B:40:ARG:CG	2:B:155:LEU:HG	2.49	0.41
2:B:230:ARG:HG2	2:B:230:ARG:HH21	1.85	0.41
8:H:51:ARG:HA	8:H:51:ARG:HD3	1.87	0.41
1:A:121:ASN:HD21	1:A:125:ILE:HD12	1.85	0.41
1:A:365:ARG:HD2	2:B:72:GLU:OE1	2.21	0.41
3:C:130:LEU:HD13	3:C:182:LEU:HB3	2.02	0.41
19:D:731:CDL:H112	19:D:731:CDL:HA4	1.56	0.41
13:A:721:UMQ:HG1	13:A:721:UMQ:HJ1	1.78	0.41
1:A:91:LEU:HD23	1:A:106:VAL:HG11	2.02	0.41
2:B:22:ARG:HH12	2:B:332:VAL:HB	1.85	0.41
2:B:24:ALA:HB3	2:B:191:ASN:HD21	1.86	0.41
17:C:710:3PE:H372	17:C:710:3PE:H3A2	1.84	0.41
4:D:223:ILE:HG12	4:D:225:MET:H	1.86	0.41
5:E:72:LYS:HZ3	9:I:29:GLN:HE22	1.67	0.41
2:B:255:VAL:HG12	2:B:321:THR:HG21	2.02	0.41
10:J:93:THR:HA	10:J:117:THR:HA	2.02	0.41
1:A:374:LEU:HA	1:A:374:LEU:HD12	1.86	0.41
3:C:182:LEU:HD12	3:C:182:LEU:HA	1.88	0.41
4:D:227:ARG:HH11	4:D:244:THR:HG21	1.86	0.41
1:A:37:VAL:HG13	1:A:207:VAL:HG22	2.03	0.41
2:B:238:VAL:HG13	2:B:356:VAL:HB	2.03	0.41
2:B:227:GLU:HB2	2:B:352:ASN:OD1	2.21	0.41
4:D:286:TRP:CD2	5:E:59:MET:HG3	2.55	0.41
2:B:175:PHE:CZ	2:B:179:VAL:HG21	2.56	0.41
2:B:265:SER:OG	2:B:267:LEU:HD12	2.21	0.41
1:A:344:ILE:HG21	1:A:448:ILE:HD12	2.03	0.41
3:C:206:SER:OG	16:C:706:UQ6:H3M1	2.21	0.41
4:D:92:ARG:HD2	4:D:250:ASP:OD2	2.20	0.41
4:D:289:LYS:HB2	8:H:37:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:36:TYR:OH	11:K:89:GLN:NE2	2.54	0.41
16:C:706:UQ6:H101	16:C:706:UQ6:H121	1.50	0.40
16:C:706:UQ6:H201	16:C:706:UQ6:H222	1.67	0.40
4:D:126:ARG:O	4:D:130:GLU:HG3	2.21	0.40
3:C:237:MET:HG2	12:D:714:3PH:H292	2.04	0.40
18:D:715:PC1:H121	18:D:715:PC1:O14	2.21	0.40
2:B:137:CYS:SG	2:B:139:VAL:HG22	2.61	0.40
4:D:208:LEU:HA	4:D:209:PRO:HD3	1.93	0.40
2:B:37:GLY:HA3	2:B:179:VAL:HG11	2.04	0.40
4:D:280:LEU:HD12	4:D:280:LEU:HA	1.94	0.40

There are no symmetry-related clashes.

## 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	429/431 (100%)	391 (91%)	33 (8%)	5 (1%)	15	27
2	B	350/352 (99%)	304 (87%)	39 (11%)	7 (2%)	9	14
3	C	383/385 (100%)	368 (96%)	14 (4%)	1 (0%)	44	66
4	D	244/246 (99%)	233 (96%)	11 (4%)	0	100	100
5	E	183/185 (99%)	168 (92%)	12 (7%)	3 (2%)	11	19
6	F	72/74 (97%)	69 (96%)	3 (4%)	0	100	100
7	G	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
8	H	91/93 (98%)	78 (86%)	9 (10%)	4 (4%)	3	3
9	I	53/55 (96%)	49 (92%)	2 (4%)	2 (4%)	4	4
10	J	125/127 (98%)	114 (91%)	8 (6%)	3 (2%)	7	11
11	K	105/107 (98%)	88 (84%)	11 (10%)	6 (6%)	2	2
All	All	2158/2180 (99%)	1983 (92%)	144 (7%)	31 (1%)	13	23

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	152	ARG
2	B	335	PRO
3	C	223	SER
8	H	93	ASN
11	K	80	PRO
2	B	22	ARG
2	B	153	LYS
5	E	46	ASN
1	A	44	PRO
1	A	227	ASN
2	B	57	GLN
5	E	103	LEU
8	H	37	LEU
9	I	12	LYS
9	I	13	ARG
10	J	65	LYS
11	K	31	ASN
11	K	51	THR
1	A	228	LEU
5	E	102	PRO
8	H	38	GLN
11	K	78	LEU
2	B	333	SER
1	A	230	LEU
10	J	32	GLY
10	J	90	ASP
11	K	16	GLY
1	A	35	GLY
8	H	40	ILE
2	B	210	PRO
11	K	68	GLY

### 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%)	343 (93%)	27 (7%)	16	31
2	B	301/301 (100%)	277 (92%)	24 (8%)	14	27
3	C	338/338 (100%)	316 (94%)	22 (6%)	20	37
4	D	204/204 (100%)	196 (96%)	8 (4%)	37	63
5	E	151/151 (100%)	148 (98%)	3 (2%)	60	84
6	F	67/67 (100%)	63 (94%)	4 (6%)	22	41
7	G	109/109 (100%)	105 (96%)	4 (4%)	39	66
8	H	77/77 (100%)	77 (100%)	0	100	100
9	I	45/45 (100%)	42 (93%)	3 (7%)	19	35
10	J	112/112 (100%)	104 (93%)	8 (7%)	17	32
11	K	93/93 (100%)	85 (91%)	8 (9%)	12	23
All	All	1867/1867 (100%)	1756 (94%)	111 (6%)	23	42

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	66	ASN
1	A	109	LEU
1	A	115	LYS
1	A	120	LEU
1	A	126	GLN
1	A	150	ASP
1	A	153	ASP
1	A	164	LEU
1	A	172	THR
1	A	173	PRO
1	A	179	ARG
1	A	183	GLU
1	A	227	ASN
1	A	239	LYS
1	A	241	LYS
1	A	252	ARG
1	A	261	ILE
1	A	289	ASN
1	A	306	ILE
1	A	330	PHE
1	A	336	ASN
1	A	343	LEU

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Mol	Chain	Res	Type
1	A	361	THR
1	A	370	LEU
1	A	390	LEU
1	A	443	LEU
2	B	17	LEU
2	B	30	THR
2	B	31	LEU
2	B	40	ARG
2	B	43	THR
2	B	53	ARG
2	B	54	PHE
2	B	62	ARG
2	B	107	ASP
2	B	128	ARG
2	B	144	ASP
2	B	146	LEU
2	B	169	LEU
2	B	193	VAL
2	B	215	LEU
2	B	267	LEU
2	B	312	LYS
2	B	330	GLU
2	B	337	GLU
2	B	338	LEU
2	B	345	ASP
2	B	347	LYS
2	B	360	SER
2	B	362	LEU
3	C	5	LYS
3	C	35	LEU
3	C	38	LEU
3	C	79	ARG
3	C	81	LEU
3	C	89	PHE
3	C	99	LYS
3	C	101	LEU
3	C	182	LEU
3	C	184	TYR
3	C	185	LEU
3	C	218	ARG
3	C	223	SER
3	C	238	LEU

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Mol	Chain	Res	Type
3	C	269	ILE
3	C	292	VAL
3	C	312	VAL
3	C	321	LEU
3	C	336	LEU
3	C	350	LEU
3	C	377	LEU
3	C	382	ARG
4	D	69	LEU
4	D	109	ARG
4	D	113	ARG
4	D	244	THR
4	D	251	VAL
4	D	256	ASN
4	D	280	LEU
4	D	283	LEU
5	E	91	MET
5	E	107	VAL
5	E	211	LYS
6	F	77	GLN
6	F	94	LEU
6	F	117	LEU
6	F	130	LEU
7	G	16	LEU
7	G	30	ASN
7	G	86	HIS
7	G	127	LYS
9	I	14	ASN
9	I	18	VAL
9	I	48	LEU
10	J	39	ARG
10	J	51	TYR
10	J	54	ASN
10	J	61	ASN
10	J	66	ASP
10	J	68	LEU
10	J	79	PHE
10	J	89	GLU
11	K	18	ARG
11	K	33	LEU
11	K	38	GLN
11	K	81	GLU

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Mol	Chain	Res	Type
11	K	82	ASP
11	K	92	ILE
11	K	93	LYS
11	K	107	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	61	ASN
1	A	63	ASN
1	A	66	ASN
1	A	67	ASN
1	A	102	GLN
1	A	121	ASN
1	A	156	HIS
1	A	171	ASN
1	A	199	ASN
1	A	200	HIS
1	A	227	ASN
1	A	274	ASN
1	A	283	GLN
1	A	289	ASN
1	A	298	GLN
1	A	314	ASN
1	A	317	HIS
1	A	336	ASN
1	A	350	GLN
1	A	385	ASN
1	A	388	ASN
1	A	429	GLN
1	A	438	GLN
2	B	49	HIS
2	B	52	ASN
2	B	55	ASN
2	B	191	ASN
2	B	246	ASN
2	B	252	GLN
2	B	258	ASN
3	C	14	ASN
3	C	22	GLN
3	C	43	GLN

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Mol	Chain	Res	Type
3	C	173	ASN
3	C	202	HIS
3	C	208	ASN
3	C	253	HIS
3	C	332	ASN
4	D	78	HIS
4	D	79	ASN
4	D	127	ASN
4	D	256	ASN
4	D	303	ASN
5	E	38	ASN
5	E	97	ASN
5	E	106	ASN
5	E	184	HIS
6	F	77	GLN
7	G	30	ASN
7	G	31	GLN
7	G	53	ASN
7	G	57	GLN
7	G	79	HIS
9	I	14	ASN
9	I	29	GLN
10	J	54	ASN
10	J	59	ASN
10	J	61	ASN
10	J	77	ASN
10	J	78	GLN
10	J	114	GLN
11	K	31	ASN
11	K	34	ASN
11	K	89	GLN
11	K	91	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

13 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	3PH	A	713	-	39,39,47	1.15	3 (7%)	43,44,52	1.61	5 (11%)
13	UMQ	A	721	-	35,35,35	1.04	2 (5%)	46,46,46	1.74	8 (17%)
14	HEM	C	701	3	28,50,50	1.76	5 (17%)	17,82,82	1.17	2 (11%)
14	HEM	C	702	3	28,50,50	1.52	5 (17%)	17,82,82	1.45	5 (29%)
15	DBT	C	705	-	17,20,20	1.23	2 (11%)	13,27,27	0.85	0
16	UQ6	C	706	-	43,43,43	3.14	18 (41%)	52,55,55	2.14	14 (26%)
17	3PE	C	710	-	46,46,50	1.14	7 (15%)	48,51,55	1.30	4 (8%)
17	3PE	C	711	-	39,39,50	0.82	1 (2%)	41,44,55	1.05	2 (4%)
14	HEM	D	703	4	28,50,50	1.68	5 (17%)	17,82,82	1.08	1 (5%)
12	3PH	D	714	-	37,37,47	1.03	1 (2%)	41,42,52	1.61	9 (21%)
18	PC1	D	715	-	37,37,53	2.00	8 (21%)	42,45,61	1.59	8 (19%)
19	CDL	D	731	-	75,75,99	1.62	14 (18%)	77,87,111	1.42	7 (9%)
20	FES	E	704	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	3PH	A	713	-	-	0/41/41/49	0/0/0/0
13	UMQ	A	721	-	-	0/20/60/60	0/2/2/2
14	HEM	C	701	3	-	0/6/54/54	0/0/8/8
14	HEM	C	702	3	-	0/6/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	DBT	C	705	-	-	0/7/27/27	0/2/2/2
16	UQ6	C	706	-	-	0/39/39/39	0/1/1/1
17	3PE	C	710	-	-	0/50/50/54	0/0/0/0
17	3PE	C	711	-	-	0/43/43/54	0/0/0/0
14	HEM	D	703	4	-	0/6/54/54	0/0/8/8
12	3PH	D	714	-	-	0/39/39/49	0/0/0/0
18	PC1	D	715	-	-	1/41/41/57	0/0/0/0
19	CDL	D	731	-	-	2/86/86/110	0/0/0/0
20	FES	E	704	5	-	0/0/4/4	0/1/1/1

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	731	CDL	OA8-CA6	-5.23	1.33	1.45
16	C	706	UQ6	O2-C2	-5.00	1.25	1.37
14	C	701	HEM	C3C-CAC	-4.67	1.38	1.47
16	C	706	UQ6	O5-C5	-4.12	1.27	1.37
14	D	703	HEM	C3B-C2B	-4.02	1.35	1.40
13	A	721	UMQ	C3-C2	-4.00	1.42	1.52
19	D	731	CDL	OA6-CA4	-3.86	1.36	1.46
14	D	703	HEM	C3C-C2C	-3.69	1.35	1.40
14	C	702	HEM	C3B-CAB	-3.63	1.40	1.47
19	D	731	CDL	OA5-CA3	-3.55	1.30	1.44
14	C	701	HEM	C3C-C2C	-3.50	1.35	1.40
12	D	714	3PH	O31-C3	-3.45	1.37	1.45
14	C	701	HEM	C3B-CAB	-3.41	1.41	1.47
14	C	702	HEM	C3C-C2C	-3.38	1.35	1.40
19	D	731	CDL	OB2-CB2	-3.36	1.31	1.44
19	D	731	CDL	CA3-CA4	-3.28	1.41	1.50
14	C	702	HEM	C3C-CAC	-2.93	1.41	1.47
19	D	731	CDL	OA9-CA7	-2.93	1.13	1.22
14	C	702	HEM	C3B-C2B	-2.88	1.36	1.40
15	C	705	DBT	C4A-C4	-2.81	1.46	1.49
14	C	701	HEM	C3B-C2B	-2.75	1.36	1.40
16	C	706	UQ6	C17-C18	-2.57	1.41	1.50
15	C	705	DBT	C7A-C7	-2.51	1.43	1.50
17	C	710	3PE	O11-C1	-2.40	1.35	1.44
17	C	710	3PE	O32-C31	-2.33	1.15	1.22
18	D	715	PC1	C1-C2	-2.27	1.44	1.50
19	D	731	CDL	OB5-CB3	-2.20	1.36	1.44
17	C	711	3PE	O21-C2	-2.06	1.41	1.46
13	A	721	UMQ	O5'-C5'	-2.01	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	731	CDL	C31-CA7	2.02	1.56	1.50
17	C	710	3PE	C3-C2	2.03	1.56	1.50
16	C	706	UQ6	C11-C9	2.06	1.55	1.51
19	D	731	CDL	CA2-C1	2.12	1.59	1.51
14	C	702	HEM	CBB-CAB	2.16	1.44	1.28
19	D	731	CDL	CB3-CB4	2.16	1.56	1.50
17	C	710	3PE	C1-C2	2.16	1.56	1.50
19	D	731	CDL	OB8-CB7	2.19	1.39	1.33
18	D	715	PC1	O32-C31	2.22	1.29	1.22
14	D	703	HEM	C3C-CAC	2.24	1.52	1.47
17	C	710	3PE	P-O14	2.24	1.59	1.50
17	C	710	3PE	O31-C31	2.32	1.40	1.33
16	C	706	UQ6	C15-C14	2.36	1.56	1.50
16	C	706	UQ6	C25-C24	2.37	1.56	1.50
18	D	715	PC1	C3-C2	2.43	1.57	1.50
18	D	715	PC1	C32-C31	2.46	1.57	1.50
19	D	731	CDL	O1-C1	2.47	1.50	1.43
12	A	713	3PH	C32-C31	2.49	1.57	1.50
16	C	706	UQ6	C13-C14	2.56	1.39	1.33
18	D	715	PC1	O22-C21	2.59	1.30	1.22
16	C	706	UQ6	C23-C24	2.60	1.39	1.33
12	A	713	3PH	C3-C2	2.66	1.58	1.50
18	D	715	PC1	P-O14	2.74	1.61	1.50
19	D	731	CDL	CB2-C1	2.77	1.61	1.51
16	C	706	UQ6	C8-C9	2.79	1.39	1.33
19	D	731	CDL	OA6-CA5	2.89	1.42	1.34
16	C	706	UQ6	C28-C29	2.90	1.40	1.33
16	C	706	UQ6	C31-C29	2.92	1.57	1.51
14	C	701	HEM	CMC-C2C	2.93	1.57	1.51
14	D	703	HEM	CBB-CAB	3.48	1.53	1.28
14	D	703	HEM	CBC-CAC	3.49	1.53	1.28
12	A	713	3PH	C1-C2	3.51	1.60	1.50
16	C	706	UQ6	C33-C34	3.55	1.42	1.32
17	C	710	3PE	O21-C21	3.56	1.44	1.34
16	C	706	UQ6	C2-C1	3.96	1.48	1.40
16	C	706	UQ6	O3-C3	4.76	1.47	1.38
16	C	706	UQ6	C2-C3	4.97	1.47	1.39
18	D	715	PC1	O31-C31	6.16	1.51	1.33
18	D	715	PC1	O21-C21	7.03	1.54	1.34
16	C	706	UQ6	C5-C6	7.41	1.51	1.40
16	C	706	UQ6	C5-C4	7.41	1.51	1.39
16	C	706	UQ6	C7-C6	10.44	1.63	1.51

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	721	UMQ	CA-O1'-C1'	-7.77	100.54	113.87
19	D	731	CDL	CB4-OB6-CB5	-6.53	102.45	117.88
18	D	715	PC1	C3-C2-C1	-4.74	101.17	111.86
19	D	731	CDL	CA6-CA4-CA3	-4.13	102.55	111.86
17	C	710	3PE	C2-O21-C21	-4.09	108.21	117.88
18	D	715	PC1	C2-O21-C21	-3.98	108.48	117.88
19	D	731	CDL	CA4-OA6-CA5	-3.83	108.83	117.88
16	C	706	UQ6	C1M-C1-C2	-3.62	114.30	120.54
12	A	713	3PH	C3-C2-C1	-3.51	103.94	111.86
12	D	714	3PH	C3-C2-C1	-3.35	104.29	111.86
17	C	711	3PE	C2-O21-C21	-3.35	109.97	117.88
12	D	714	3PH	C38-C37-C36	-3.26	97.66	114.45
12	A	713	3PH	O14-P-O11	-3.04	98.64	106.73
14	C	702	HEM	CMA-C3A-C4A	-3.00	123.85	128.46
13	A	721	UMQ	C3'-C4'-C5'	-2.89	104.75	110.88
19	D	731	CDL	CB6-CB4-CB3	-2.88	105.35	111.86
18	D	715	PC1	C3-O31-C31	-2.86	108.54	117.13
13	A	721	UMQ	O1-C1-O5	-2.80	103.89	110.70
12	D	714	3PH	O31-C3-C2	-2.62	102.08	108.66
14	D	703	HEM	CMD-C2D-C1D	-2.57	124.51	128.46
14	C	701	HEM	CMD-C2D-C1D	-2.54	124.56	128.46
12	D	714	3PH	O14-P-O11	-2.51	100.06	106.73
12	D	714	3PH	O31-C31-C32	-2.46	104.73	111.90
13	A	721	UMQ	O3'-C3'-C2'	-2.46	105.00	110.36
14	C	702	HEM	CBD-CAD-C3D	-2.44	107.81	112.47
13	A	721	UMQ	CD-CC-CB	-2.43	101.92	114.45
17	C	710	3PE	C3E-C3D-C3C	-2.37	102.24	114.45
16	C	706	UQ6	C15-C14-C16	-2.35	111.21	115.29
18	D	715	PC1	C37-C36-C35	-2.33	102.46	114.45
16	C	706	UQ6	C20-C19-C18	-2.29	117.57	123.69
16	C	706	UQ6	C36-C34-C35	-2.19	109.49	114.60
19	D	731	CDL	CB2-C1-CA2	-2.18	106.19	112.73
13	A	721	UMQ	C6'-C5'-C4'	-2.17	107.31	113.24
13	A	721	UMQ	C1-O5-C5	-2.12	109.72	113.72
17	C	711	3PE	C29-C28-C27	-2.09	103.69	114.45
18	D	715	PC1	O21-C21-C22	-2.04	107.31	111.55
17	C	710	3PE	O31-C3-C2	-2.02	103.57	108.66
19	D	731	CDL	OA4-PA1-OA3	-2.00	101.91	112.28
18	D	715	PC1	C23-C22-C21	2.06	121.10	113.58
16	C	706	UQ6	C11-C9-C8	2.09	125.37	121.10
16	C	706	UQ6	C16-C14-C13	2.12	125.44	121.10
14	C	702	HEM	CMA-C3A-C2A	2.19	129.06	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	702	HEM	CMB-C2B-C3B	2.20	128.97	124.89
12	D	714	3PH	O31-C31-O32	2.27	129.19	123.55
16	C	706	UQ6	C1M-C1-C6	2.47	123.96	120.43
19	D	731	CDL	OB4-PB2-OB2	2.57	120.30	108.14
18	D	715	PC1	O21-C2-C1	2.63	118.01	108.44
14	C	702	HEM	CMC-C2C-C3C	2.64	129.79	124.89
16	C	706	UQ6	C2-C1-C6	2.72	121.74	118.64
18	D	715	PC1	C11-C12-N	2.73	125.13	115.86
12	D	714	3PH	O11-P-O12	2.78	114.28	106.47
16	C	706	UQ6	C11-C12-C13	2.84	121.69	111.97
14	C	701	HEM	CMB-C2B-C3B	2.98	130.43	124.89
13	A	721	UMQ	O1'-CA-CB	3.04	120.54	109.68
16	C	706	UQ6	C6-C7-C8	3.16	117.01	112.17
17	C	710	3PE	C3-C2-C1	3.44	119.61	111.86
12	D	714	3PH	O13-P-O11	3.57	116.24	106.73
12	A	713	3PH	O13-P-O11	3.63	116.41	106.73
12	A	713	3PH	O11-P-O12	3.66	116.75	106.47
16	C	706	UQ6	C21-C19-C18	3.95	129.18	121.10
12	D	714	3PH	P-O11-C1	4.41	130.43	118.30
16	C	706	UQ6	C4M-O4-C4	4.56	127.30	114.81
16	C	706	UQ6	C17-C18-C19	5.14	140.59	127.68
12	A	713	3PH	P-O11-C1	5.34	133.00	118.30
16	C	706	UQ6	C3M-O3-C3	7.70	135.91	114.81

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	D	731	CDL	CA4-OA6-CA5-OA7
19	D	731	CDL	CA4-OA6-CA5-C11
18	D	715	PC1	P-O13-C11-C12

There are no ring outliers.

10 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	713	3PH	4	0
13	A	721	UMQ	2	0
14	C	702	HEM	1	0
15	C	705	DBT	1	0
16	C	706	UQ6	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	C	710	3PE	3	0
12	D	714	3PH	3	0
18	D	715	PC1	3	0
19	D	731	CDL	5	0
20	E	704	FES	1	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.