



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:30 PM GMT

PDB ID : 1P84
Title : HDBT inhibited Yeast Cytochrome bc1 Complex
Authors : Palsdottir, H.; Lojero, C.G.; Trumpower, B.L.; Hunte, C.
Deposited on : 2003-05-06
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
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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

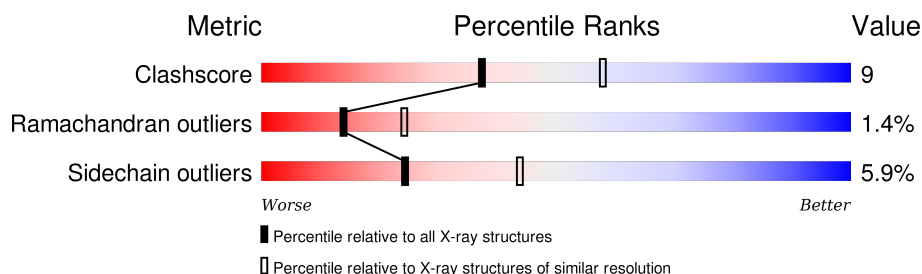
1 Overall quality at a glance ⓘ

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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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 ≥ 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	 85% 13% •
9	I	55	 85% 11% •
10	J	127	 69% 26% 5%
11	K	107	 60% 35% 6%

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.

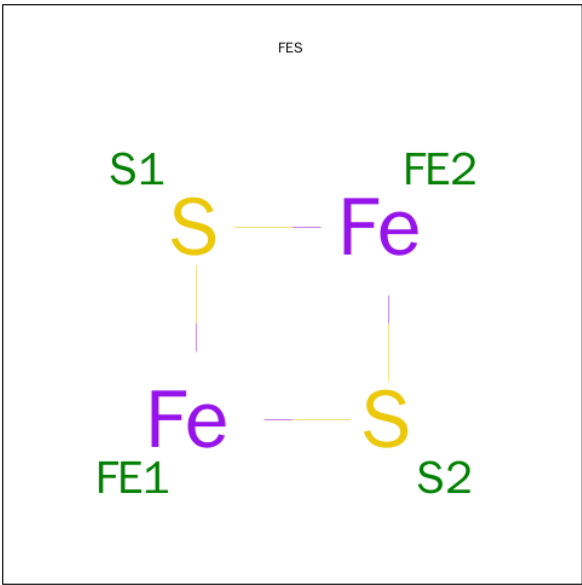
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	107	Total	C	N	O	S	0	0	0
			842	536	141	163	2			

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



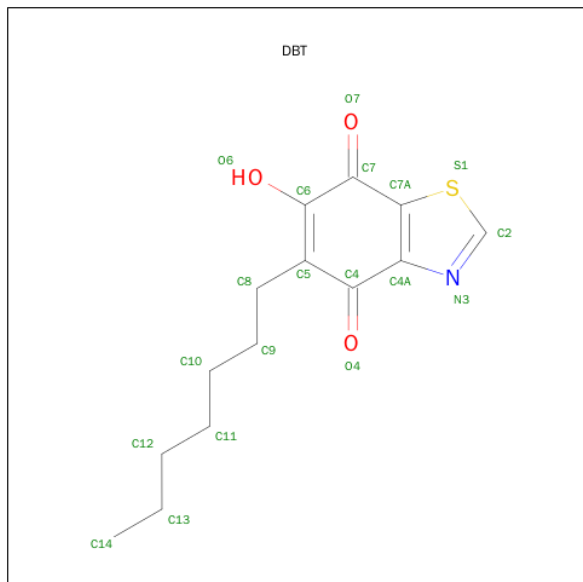
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



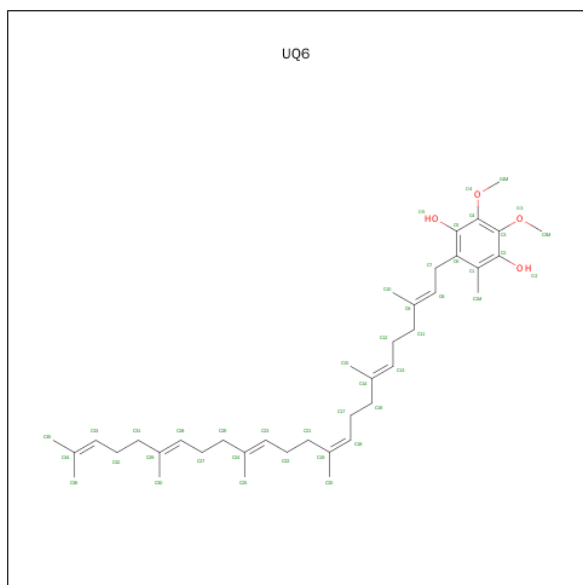
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	E	1	Total	Fe	S	0	0
			4	2	2		

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



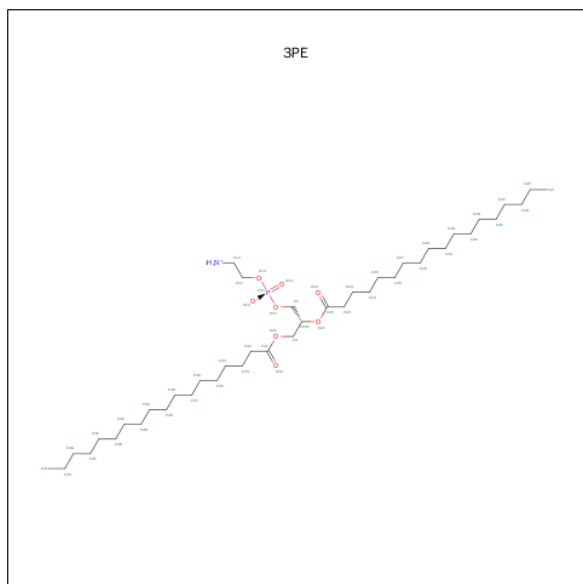
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total	C	N	O	S	0	0
			19	14	1	3	1		

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



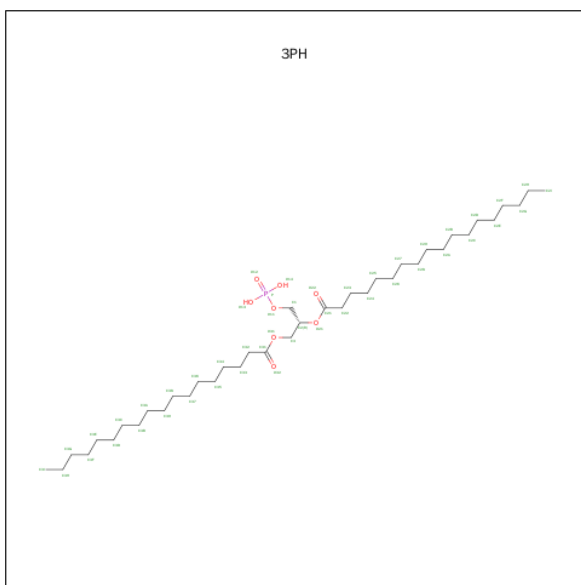
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	C	1	Total	C	O	0	0
			43	39	4		

- Molecule 16 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



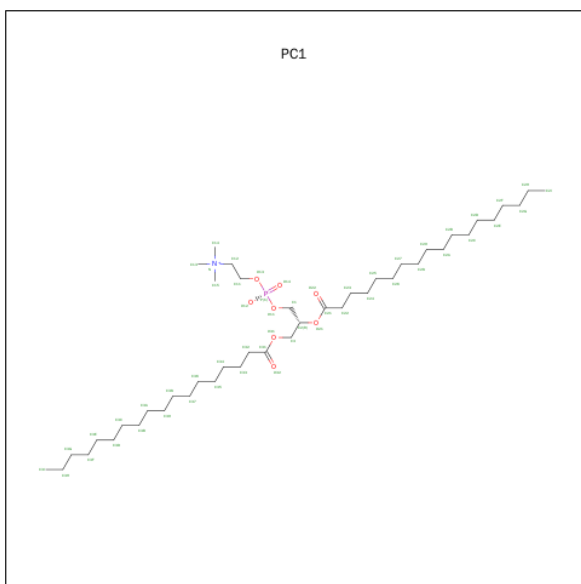
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	C	1	Total	C	N	O	P	0	0
			47	37	1	8	1		
16	C	1	Total	C	N	O	P	0	0
			40	30	1	8	1		

- Molecule 17 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$).



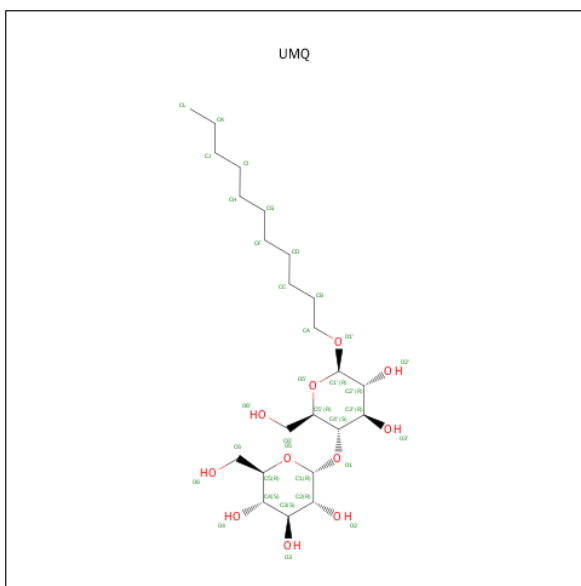
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	A	1	Total	C	O	P	0	0
			40	31	8	1		
17	D	1	Total	C	O	P	0	0
			38	29	8	1		

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



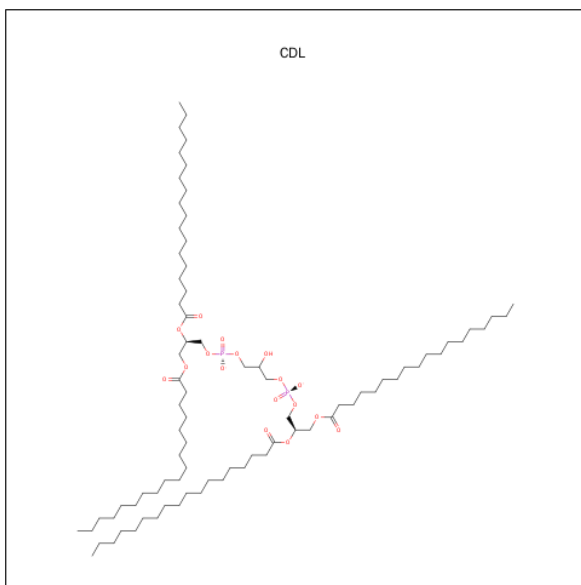
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	D	1	Total	C	N	O	P	0	0
			38	28	1	8	1		

- Molecule 19 is UNDECYL-MALTOSE (three-letter code: UMQ) (formula: $C_{23}H_{44}O_{11}$).



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

- Molecule 20 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

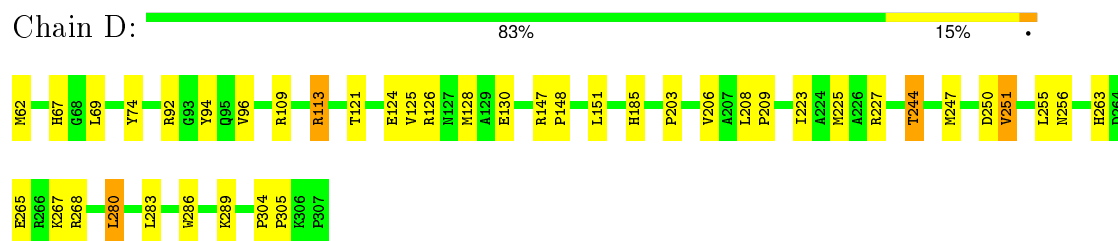


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	D	1	Total	C	O	P	0	0
			76	57	17	2		

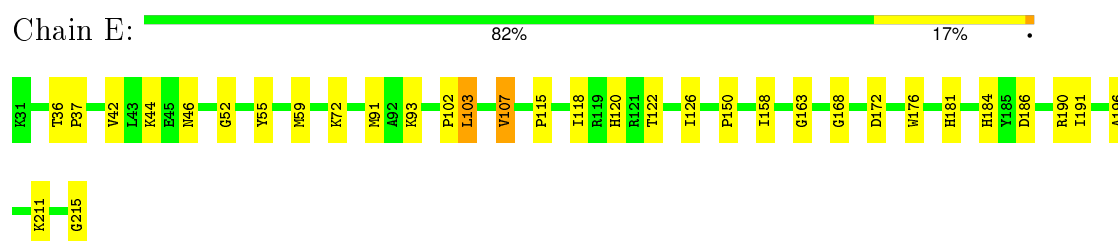
- Molecule 21 is water.

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

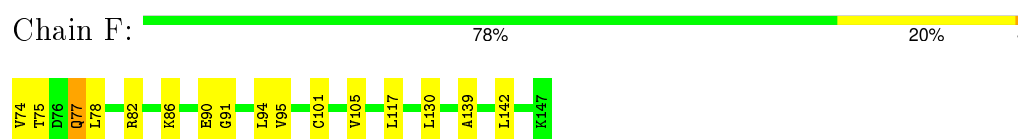
- Molecule 4: Cytochrome c1, heme protein



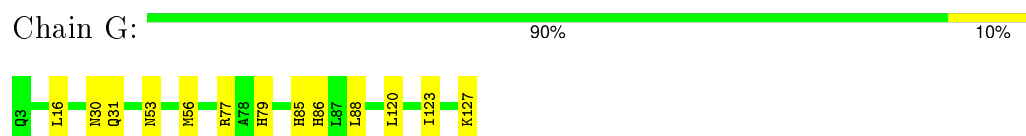
- Molecule 5: Ubiquinol-cytochrome C reductase iron-sulfur subunit



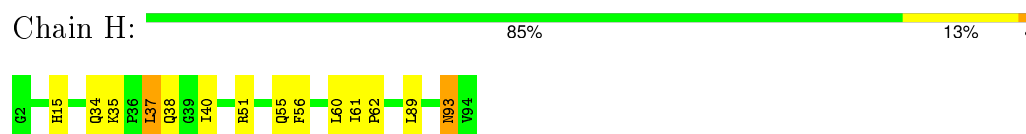
- Molecule 6: Ubiquinol-cytochrome C reductase complex 17 kDa protein



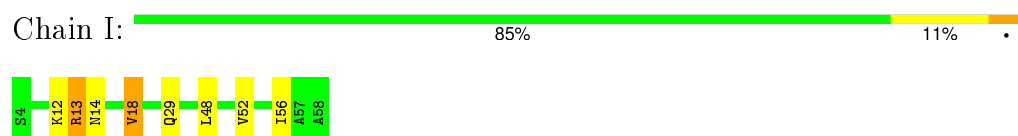
- Molecule 7: Ubiquinol-cytochrome C reductase complex 14 kDa protein



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

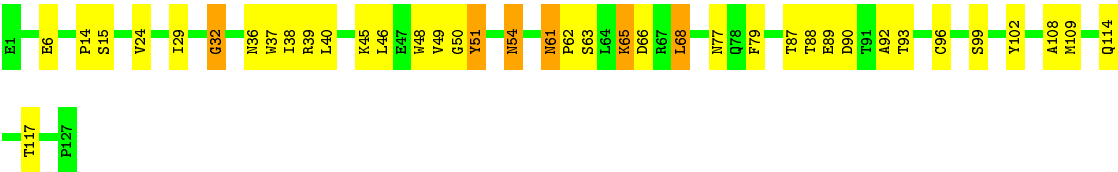


- Molecule 9: Ubiquinol-cytochrome C reductase complex 7.3 kDa protein

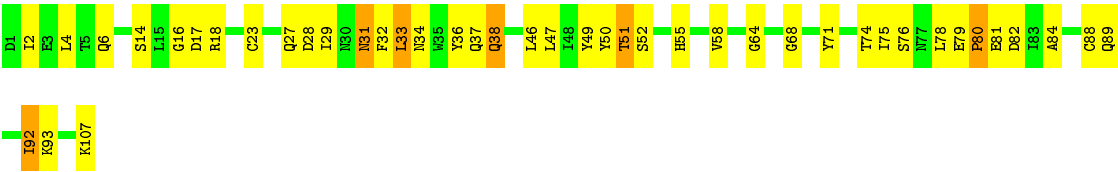
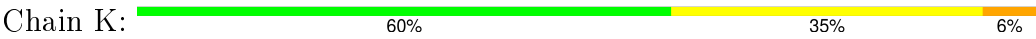


- Molecule 10: Heavy Chain (Vh) Of Fv-Fragment





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



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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 ²)	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	C	86	0	60	1	0
12	D	43	0	30	0	0
13	E	4	0	0	1	0
14	C	19	0	17	1	0
15	C	43	0	58	8	0
16	C	87	0	128	3	0
17	A	40	0	53	4	0
17	D	38	0	49	3	0
18	D	38	0	50	3	0
19	A	34	0	44	2	0
20	D	76	0	99	5	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)
15:C:706:UQ6:H1M1	15:C:706:UQ6:H103	1.31	1.10
6:F:77:GLN:H	6:F:77:GLN:HE21	1.01	0.98
16: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
15:C:706:UQ6:C10	15: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
15:C:706:UQ6:C1M	15: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
17: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
20:D:731:CDL:HB22	7:G:85:HIS:NE2	2.03	0.74
20:D:731:CDL:H351	20: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	14: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	20: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
17:A:713:3PH:H282	3:C:230:LEU:HD13	1.81	0.63
2:B:65:LEU:O	2:B:69:ARG:HG2	1.99	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
11:K:29:ILE:HG22	11:K:92:ILE:HD12	1.81	0.61
1:A:172:THR:HG23	1:A:173:PRO:HD2	1.83	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
11:K:29:ILE:HA	11:K:92:ILE:HG21	1.82	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: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
2:B:24:ALA:HB3	2:B:191:ASN:ND2	2.18	0.58
1:A:46:ALA:O	1:A:47:HIS:HB2	2.03	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
7:G:77:ARG:HD2	21:G:149:HOH:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:44:LYS:NZ	5:E:52:GLY:H	2.01	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
4:D:185:HIS:ND1	18:D:715:PC1:H142	2.19	0.57
1:A:313:ASP:OD1	1:A:335:ARG:HD3	2.05	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	15: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
16: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
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
2:B:36:HIS:HB2	2:B:184:ASN:OD1	2.08	0.53
17:D:714:3PH:H2A2	17:D:714:3PH:H251	1.89	0.53
1:A:58:GLY:H	1:A:61:ASN:HD22	1.55	0.53
10:J:87:THR:HG22	10:J:88:THR:N	2.23	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
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
3:C:208:ASN:ND2	3:C:210:LEU:H	2.08	0.52
1:A:169:PHE:O	1:A:172:THR:HB	2.09	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
5:E:103:LEU:HA	5:E:120:HIS:ND1	2.26	0.51
4:D:147:ARG:HG2	4:D:148:PRO:O	2.10	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
4:D:96:VAL:HB	4:D:251:VAL:HG13	1.94	0.50
1:A:373:GLN:HG3	1:A:374:LEU:N	2.26	0.50
11:K:4:LEU:HD23	11:K:88:CYS:SG	2.51	0.50
4:D:263:HIS:NE2	4:D:267:LYS:HE3	2.26	0.50
2:B:347:LYS:HG2	2:B:348:LEU:N	2.27	0.50
3:C:175:THR:O	3:C:178:ARG:HG2	2.12	0.50
2:B:52:ASN:HD21	2:B:80:SER:C	2.15	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
19:A:721:UMQ:O2'	9:I:18:VAL:HG22	2.14	0.48
2:B:62:ARG:HH21	2:B:62:ARG:HB2	1.77	0.48
2:B:197:LEU:O	2:B:201:VAL:HG23	2.13	0.48
6:F:74:VAL:HG12	6:F:75:THR:N	2.28	0.48
2:B:26:THR:OG1	2:B:191:ASN:ND2	2.47	0.48
4:D:125:VAL:HA	4:D:128:MET:HE3	1.96	0.48
1:A:127:GLN:C	1:A:129:ALA:H	2.17	0.48
5:E:168:GLY:HA2	5:E:176:TRP:CD1	2.48	0.48
5:E:172:ASP:H	5:E:184:HIS:CD2	2.31	0.48
2:B:58:ASN:OD1	2:B:63:SER:HA	2.14	0.48
5:E:181:HIS:HB2	13:E:704:FES:S1	2.54	0.47
10:J:54:ASN:H	10:J:54:ASN:HD22	1.62	0.47
1:A:179:ARG:HG2	1:A:179:ARG:HH21	1.78	0.47
1:A:67:ASN:HD22	1:A:181:THR:HG23	1.79	0.47
2:B:52:ASN:ND2	2:B:80:SER:OG	2.47	0.47
2:B:241:ILE:HA	2:B:352:ASN:O	2.15	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
4:D:286:TRP:CD2	8:H:37:LEU:HD12	2.50	0.47
1:A:349:LYS:HA	1:A:349:LYS:HD3	1.63	0.47
11:K:74:THR:HG22	11:K:75:ILE:N	2.29	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:52:SER:HB3	11:K:64:GLY:O	2.15	0.47
2:B:21:ALA:O	2:B:22:ARG:HB2	2.14	0.47
1:A:456:ARG:HH21	1:A:456:ARG:HG3	1.80	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
17:A:713:3PH:H3B2	17: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)
11:K:2:ILE:HD12	11:K:2:ILE:N	2.29	0.46
4:D:121:THR:OG1	4:D:124:GLU:HG3	2.15	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:63:ASN:HB2	1:A:66:ASN:HD22	1.75	0.46
1:A:58:GLY:N	1:A:61:ASN:ND2	2.62	0.46
2:B:252:GLN:O	2:B:255:VAL:HG22	2.16	0.46
1:A:350:GLN:NE2	1:A:353:ARG:HD3	2.30	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:CZ	2.51	0.46
1:A:67:ASN:ND2	1:A:181:THR:HG23	2.31	0.45
1:A:86:ALA:HB2	1:A:119:PHE:CE1	2.51	0.45
10:J:45:LYS:O	10:J:45:LYS:HG3	2.16	0.45
11:K:32:PHE:CD2	11:K:92:ILE:HG22	2.43	0.45
11:K:46:LEU:HD23	11:K:55:HIS:CD2	2.51	0.45
3:C:201:LEU:HD21	15:C:706:UQ6:H3M2	1.98	0.45
10:J:61:ASN:HD22	10:J:61:ASN:C	2.19	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
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
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
1:A:49:ALA:HA	1:A:212:GLY:HA3	1.98	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
20:D:731:CDL:HB22	7:G:85:HIS:HE2	1.82	0.44
10:J:29:ILE:HG12	10:J:77:ASN:ND2	2.32	0.44
2:B:69:ARG:O	2:B:73:LEU:HD23	2.17	0.44
10:J:14:PRO:O	10:J:15:SER:HB3	2.17	0.44
8:H:15:HIS:HB3	21:H:106:HOH:O	2.16	0.44
10:J:49:VAL:CG1	10:J:68:LEU:HD23	2.47	0.44
2:B:228:GLU:HA	2:B:353:TYR:O	2.17	0.44
1:A:317:HIS:HE1	1:A:351:TRP:NE1	2.05	0.44
5:E:191:ILE:CD1	5:E:196:ALA:HB3	2.47	0.44
1:A:121:ASN:ND2	1:A:125:ILE:HD12	2.33	0.44
2:B:29:SER:HA	2:B:191:ASN:HB3	2.00	0.44
2:B:155:LEU:HD12	2:B:155:LEU:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:LEU:N	2:B:155:LEU:HD12	2.32	0.44
4:D:203:PRO:HG2	4:D:206:VAL:CG2	2.48	0.44
1:A:142:LYS:NZ	1:A:142:LYS:HB2	2.33	0.44
1:A:58:GLY:N	1:A:61:ASN:HD22	2.15	0.44
1:A:289:ASN:ND2	1:A:289:ASN:C	2.70	0.44
4:D:304:PRO:HA	4:D:305:PRO:HD3	1.84	0.44
12:C:702:HEM:HMC2	12:C:702:HEM:HBC2	2.00	0.44
1:A:29:VAL:HG11	1:A:400:LYS:HB3	1.99	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
5:E:186:ASP:OD2	5:E:190:ARG:HD2	2.18	0.43
2:B:141:SER:O	2:B:145:GLN:HG2	2.17	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
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:239:ALA:HB1	2:B:301:ILE:HD12	2.00	0.43
10:J:38:ILE:O	10:J:38:ILE:HG13	2.19	0.43
2:B:294:SER:HB3	2:B:358:ASP:HB3	2.01	0.43
17: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
5:E:72:LYS:HZ2	9:I:29:GLN:NE2	2.16	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
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
11:K:79:GLU:HA	11:K:80:PRO:HA	1.87	0.42
4:D:255:LEU:HD23	4:D:255:LEU:HA	1.88	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
10:J:29:ILE:H	10:J:77:ASN:ND2	2.15	0.42
5:E:36:THR:HA	5:E:37:PRO:HD2	1.92	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)
11:K:4:LEU:CD2	11:K:88:CYS:SG	3.08	0.42
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:75:ILE:HG22	11:K:76:SER:N	2.35	0.42
10:J:38:ILE:HD12	10:J:46:LEU:HD22	2.02	0.42
2:B:150:THR:HG22	2:B:352:ASN:ND2	2.35	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
8:H:51:ARG:HA	8:H:51:ARG:HD3	1.87	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
20:D:731:CDL:H112	20:D:731:CDL:HA4	1.56	0.41
1:A:121:ASN:HD21	1:A:125:ILE:HD12	1.85	0.41
3:C:130:LEU:HD13	3:C:182:LEU:HB3	2.02	0.41
1:A:365:ARG:HD2	2:B:72:GLU:OE1	2.21	0.41
16:C:710:3PE:H372	16:C:710:3PE:H3A2	1.84	0.41
2:B:24:ALA:HB3	2:B:191:ASN:HD21	1.86	0.41
19:A:721:UMQ:HG1	19:A:721:UMQ:HJ1	1.78	0.41
2:B:22:ARG:HH12	2:B:332:VAL:HB	1.85	0.41
5:E:72:LYS:HZ3	9:I:29:GLN:HE22	1.67	0.41
4:D:223:ILE:HG12	4:D:225:MET:H	1.86	0.41
1:A:91:LEU:HD23	1:A:106:VAL:HG11	2.02	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
2:B:265:SER:OG	2:B:267:LEU:HD12	2.21	0.41
4:D:286:TRP:CD2	5:E:59:MET:HG3	2.55	0.41
2:B:227:GLU:HB2	2:B:352:ASN:OD1	2.21	0.41
2:B:175:PHE:CZ	2:B:179:VAL:HG21	2.56	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
3:C:206:SER:OG	15:C:706:UQ6:H3M1	2.21	0.41
4:D:289:LYS:HB2	8:H:37:LEU:HD13	2.03	0.41
11:K:36:TYR:OH	11:K:89:GLN:NE2	2.54	0.41
4:D:92:ARG:HD2	4:D:250:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ILE:HG21	1:A:448:ILE:HD12	2.03	0.41
15:C:706:UQ6:H101	15:C:706:UQ6:H121	1.50	0.40
15:C:706:UQ6:H201	15:C:706:UQ6:H222	1.67	0.40
3:C:237:MET:HG2	17:D:714:3PH:H292	2.04	0.40
18:D:715:PC1:H121	18:D:715:PC1:O14	2.21	0.40
4:D:126:ARG:O	4:D:130:GLU:HG3	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%)	16	29
2	B	350/352 (99%)	304 (87%)	39 (11%)	7 (2%)	9	15
3	C	383/385 (100%)	368 (96%)	14 (4%)	1 (0%)	46	68
4	D	244/246 (99%)	233 (96%)	11 (4%)	0	100	100
5	E	183/185 (99%)	168 (92%)	12 (7%)	3 (2%)	12	21
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	5
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%)	14	24

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%)	17	32
2	B	301/301 (100%)	277 (92%)	24 (8%)	15	28
3	C	338/338 (100%)	316 (94%)	22 (6%)	21	39
4	D	204/204 (100%)	196 (96%)	8 (4%)	39	66
5	E	151/151 (100%)	148 (98%)	3 (2%)	63	86
6	F	67/67 (100%)	63 (94%)	4 (6%)	24	43
7	G	109/109 (100%)	105 (96%)	4 (4%)	41	68
8	H	77/77 (100%)	77 (100%)	0	100	100
9	I	45/45 (100%)	42 (93%)	3 (7%)	20	37
10	J	112/112 (100%)	104 (93%)	8 (7%)	18	34
11	K	93/93 (100%)	85 (91%)	8 (9%)	13	24
All	All	1867/1867 (100%)	1756 (94%)	111 (6%)	24	44

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
17	3PH	A	713	-	39,39,47	1.16	4 (10%)	42,44,52	1.39	5 (11%)
19	UMQ	A	721	-	35,35,35	1.01	1 (2%)	46,46,46	1.70	9 (19%)
12	HEM	C	701	3	30,50,50	2.95	11 (36%)	24,82,82	2.09	6 (25%)
12	HEM	C	702	3	30,50,50	2.85	9 (30%)	24,82,82	2.53	10 (41%)
14	DBT	C	705	-	16,20,20	1.25	2 (12%)	12,27,27	0.87	0
15	UQ6	C	706	-	43,43,43	3.18	19 (44%)	52,55,55	2.32	16 (30%)
16	3PE	C	710	-	46,46,50	1.14	7 (15%)	47,51,55	1.29	3 (6%)
16	3PE	C	711	-	39,39,50	0.84	2 (5%)	40,44,55	1.04	2 (5%)
12	HEM	D	703	4	30,50,50	2.54	8 (26%)	24,82,82	3.15	8 (33%)
17	3PH	D	714	-	37,37,47	1.03	1 (2%)	40,42,52	1.45	9 (22%)
18	PC1	D	715	-	37,37,53	1.96	9 (24%)	41,45,61	1.59	6 (14%)
20	CDL	D	731	-	75,75,99	1.59	13 (17%)	77,87,111	1.39	6 (7%)
13	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
17	3PH	A	713	-	-	0/41/41/49	0/0/0/0
19	UMQ	A	721	-	-	0/20/60/60	0/2/2/2
12	HEM	C	701	3	-	0/10/54/54	0/0/8/8
12	HEM	C	702	3	-	0/10/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	DBT	C	705	-	-	0/7/27/27	0/2/2/2
15	UQ6	C	706	-	-	0/39/39/39	0/1/1/1
16	3PE	C	710	-	-	0/50/50/54	0/0/0/0
16	3PE	C	711	-	-	0/43/43/54	0/0/0/0
12	HEM	D	703	4	-	0/10/54/54	0/0/8/8
17	3PH	D	714	-	-	0/39/39/49	0/0/0/0
18	PC1	D	715	-	-	1/41/41/57	0/0/0/0
20	CDL	D	731	-	-	2/86/86/110	0/0/0/0
13	FES	E	704	5	-	0/0/4/4	0/1/1/1

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	702	HEM	C3B-C4B	-8.32	1.44	1.51
12	C	701	HEM	C3B-C4B	-8.18	1.44	1.51
12	D	703	HEM	C3B-C4B	-7.28	1.45	1.51
12	C	701	HEM	C3C-CAC	-6.87	1.38	1.51
12	C	702	HEM	C2D-C3D	-6.41	1.35	1.54
12	C	701	HEM	C2D-C3D	-6.17	1.36	1.54
12	D	703	HEM	C2D-C3D	-6.05	1.36	1.54
12	C	702	HEM	C3B-CAB	-5.69	1.40	1.51
12	C	701	HEM	C3B-CAB	-5.45	1.41	1.51
12	D	703	HEM	C3D-C4D	-5.39	1.44	1.51
20	D	731	CDL	OA8-CA6	-5.19	1.33	1.45
12	C	701	HEM	C3D-C4D	-5.05	1.45	1.51
12	C	702	HEM	C3C-CAC	-5.03	1.41	1.51
12	C	702	HEM	C3D-C4D	-5.01	1.45	1.51
15	C	706	UQ6	O2-C2	-4.93	1.25	1.37
15	C	706	UQ6	O5-C5	-4.06	1.27	1.37
12	C	702	HEM	C2C-C1C	-3.98	1.45	1.52
20	D	731	CDL	OA6-CA4	-3.94	1.36	1.46
12	C	701	HEM	C2C-C1C	-3.92	1.45	1.52
19	A	721	UMQ	C3-C2	-3.90	1.42	1.52
12	D	703	HEM	C2C-C1C	-3.85	1.45	1.52
20	D	731	CDL	OA5-CA3	-3.44	1.30	1.44
17	D	714	3PH	O31-C3	-3.41	1.37	1.45
20	D	731	CDL	CA3-CA4	-3.27	1.41	1.50
20	D	731	CDL	OB2-CB2	-3.26	1.31	1.44
15	C	706	UQ6	C17-C18	-3.15	1.41	1.50
20	D	731	CDL	OA9-CA7	-2.95	1.13	1.22
14	C	705	DBT	C4A-C4	-2.78	1.46	1.49
14	C	705	DBT	C7A-C7	-2.51	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	701	HEM	C2B-C1B	-2.43	1.43	1.51
16	C	710	3PE	O32-C31	-2.35	1.15	1.22
16	C	710	3PE	O11-C1	-2.33	1.35	1.44
18	D	715	PC1	C1-C2	-2.26	1.44	1.50
12	C	701	HEM	C2D-C1D	-2.23	1.44	1.51
15	C	706	UQ6	C12-C13	-2.19	1.44	1.50
12	D	703	HEM	C2B-C1B	-2.15	1.44	1.51
20	D	731	CDL	OB5-CB3	-2.13	1.36	1.44
16	C	711	3PE	O21-C2	-2.10	1.41	1.46
12	C	702	HEM	C2D-C1D	-2.09	1.45	1.51
12	C	702	HEM	C2B-C1B	-2.01	1.45	1.51
12	D	703	HEM	C2D-C1D	-2.00	1.45	1.51
12	C	701	HEM	CMC-C2C	2.02	1.57	1.53
20	D	731	CDL	CA2-C1	2.02	1.59	1.51
16	C	710	3PE	C3-C2	2.04	1.56	1.50
17	A	713	3PH	P-O13	2.06	1.62	1.54
16	C	711	3PE	C12-C11	2.10	1.56	1.50
12	C	701	HEM	CBC-CAC	2.11	1.41	1.29
20	D	731	CDL	OB8-CB7	2.14	1.39	1.33
18	D	715	PC1	P-O12	2.16	1.64	1.54
20	D	731	CDL	CB3-CB4	2.17	1.56	1.50
16	C	710	3PE	C1-C2	2.17	1.56	1.50
12	C	701	HEM	CBB-CAB	2.20	1.42	1.29
18	D	715	PC1	O32-C31	2.20	1.29	1.22
16	C	710	3PE	P-O14	2.23	1.59	1.51
16	C	710	3PE	O31-C31	2.27	1.40	1.33
15	C	706	UQ6	C18-C19	2.34	1.37	1.33
18	D	715	PC1	C32-C31	2.40	1.57	1.50
20	D	731	CDL	O1-C1	2.42	1.50	1.43
17	A	713	3PH	C32-C31	2.43	1.57	1.50
18	D	715	PC1	C3-C2	2.44	1.57	1.50
15	C	706	UQ6	C15-C14	2.49	1.56	1.50
15	C	706	UQ6	C25-C24	2.50	1.56	1.50
12	C	702	HEM	CBB-CAB	2.56	1.44	1.29
18	D	715	PC1	O22-C21	2.57	1.30	1.22
20	D	731	CDL	CB2-C1	2.64	1.61	1.51
17	A	713	3PH	C3-C2	2.67	1.58	1.50
18	D	715	PC1	P-O14	2.74	1.61	1.51
20	D	731	CDL	OA6-CA5	2.80	1.42	1.34
15	C	706	UQ6	C31-C29	2.84	1.57	1.51
15	C	706	UQ6	C13-C14	3.26	1.39	1.33
15	C	706	UQ6	C23-C24	3.32	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	706	UQ6	C33-C34	3.40	1.42	1.32
15	C	706	UQ6	C2-C1	3.44	1.48	1.40
16	C	710	3PE	O21-C21	3.45	1.44	1.34
17	A	713	3PH	C1-C2	3.51	1.60	1.50
15	C	706	UQ6	C8-C9	3.56	1.39	1.33
15	C	706	UQ6	C28-C29	3.71	1.40	1.33
12	D	703	HEM	CBB-CAB	4.18	1.53	1.29
12	D	703	HEM	CBC-CAC	4.18	1.53	1.29
15	C	706	UQ6	O3-C3	4.82	1.47	1.38
15	C	706	UQ6	C2-C3	4.87	1.47	1.39
18	D	715	PC1	O31-C31	6.03	1.51	1.33
18	D	715	PC1	O21-C21	6.80	1.54	1.34
15	C	706	UQ6	C5-C4	7.27	1.51	1.39
15	C	706	UQ6	C5-C6	7.62	1.51	1.40
15	C	706	UQ6	C7-C6	9.87	1.63	1.51

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	703	HEM	C3B-CAB-CBB	-9.69	109.60	124.46
19	A	721	UMQ	CA-O1'-C1'	-7.67	100.54	113.94
12	D	703	HEM	C3C-CAC-CBC	-6.90	113.86	124.46
20	D	731	CDL	CB4-OB6-CB5	-6.43	102.45	117.89
18	D	715	PC1	C3-C2-C1	-4.66	101.17	112.07
20	D	731	CDL	CA6-CA4-CA3	-4.07	102.55	112.07
16	C	710	3PE	C2-O21-C21	-4.04	108.21	117.89
18	D	715	PC1	C2-O21-C21	-3.92	108.48	117.89
20	D	731	CDL	CA4-OA6-CA5	-3.78	108.83	117.89
17	A	713	3PH	C3-C2-C1	-3.48	103.94	112.07
15	C	706	UQ6	C1M-C1-C2	-3.35	114.30	120.36
17	D	714	3PH	C3-C2-C1	-3.33	104.29	112.07
16	C	711	3PE	C2-O21-C21	-3.30	109.97	117.89
17	D	714	3PH	C38-C37-C36	-3.27	97.66	114.53
15	C	706	UQ6	C20-C19-C18	-3.02	117.57	123.50
18	D	715	PC1	C3-O31-C31	-2.97	108.54	116.85
20	D	731	CDL	CB6-CB4-CB3	-2.87	105.35	112.07
17	A	713	3PH	O14-P-O11	-2.75	98.64	106.56
15	C	706	UQ6	C15-C14-C16	-2.75	111.21	115.41
12	C	702	HEM	CMA-C3A-C4A	-2.73	123.85	128.36
19	A	721	UMQ	C3'-C4'-C5'	-2.69	104.75	110.84
19	A	721	UMQ	O1-C1-O5	-2.68	103.89	110.68
12	C	702	HEM	CAA-C2A-C1A	-2.63	124.15	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	714	3PH	O31-C3-C2	-2.46	102.08	108.69
19	A	721	UMQ	CD-CC-CB	-2.44	101.92	114.53
16	C	710	3PE	C3E-C3D-C3C	-2.38	102.24	114.53
19	A	721	UMQ	O3'-C3'-C2'	-2.37	105.00	110.34
17	D	714	3PH	O31-C31-C32	-2.35	104.73	111.90
18	D	715	PC1	C37-C36-C35	-2.34	102.46	114.53
17	D	714	3PH	O14-P-O11	-2.26	100.06	106.56
17	D	714	3PH	O14-P-O12	-2.25	103.34	110.58
16	C	711	3PE	C29-C28-C27	-2.10	103.69	114.53
15	C	706	UQ6	C36-C34-C35	-2.10	109.49	114.64
20	D	731	CDL	CB2-C1-CA2	-2.08	106.19	112.92
19	A	721	UMQ	C1-O5-C5	-2.08	109.72	113.75
17	A	713	3PH	O13-P-O12	-2.05	103.97	110.58
19	A	721	UMQ	C6'-C5'-C4'	-2.04	107.31	113.25
19	A	721	UMQ	O6-C6-C5	2.03	118.03	111.33
15	C	706	UQ6	C31-C29-C28	2.10	125.04	121.05
17	D	714	3PH	O31-C31-O32	2.21	129.19	123.49
15	C	706	UQ6	C11-C9-C8	2.28	125.37	121.05
15	C	706	UQ6	C16-C14-C13	2.31	125.44	121.05
20	D	731	CDL	OB4-PB2-OB2	2.35	120.30	108.46
15	C	706	UQ6	C21-C22-C23	2.37	117.89	111.69
15	C	706	UQ6	C1M-C1-C6	2.38	123.96	120.42
12	C	702	HEM	CMD-C2D-C3D	2.64	126.05	114.35
19	A	721	UMQ	O1'-CA-CB	2.68	120.54	109.88
15	C	706	UQ6	C2-C1-C6	2.69	121.74	118.79
12	C	701	HEM	CMC-C2C-C3C	2.71	123.29	116.53
18	D	715	PC1	O21-C2-C1	2.74	118.01	108.36
17	D	714	3PH	O11-P-O12	2.80	114.28	107.14
18	D	715	PC1	C11-C12-N	2.83	125.13	116.03
15	C	706	UQ6	C6-C7-C8	2.83	117.01	112.32
12	D	703	HEM	C2D-C3D-C4D	3.12	106.79	101.50
12	C	702	HEM	C2D-C3D-C4D	3.15	106.83	101.50
12	D	703	HEM	CMD-C2D-C3D	3.17	128.39	114.35
12	C	701	HEM	C2D-C3D-C4D	3.21	106.95	101.50
16	C	710	3PE	C3-C2-C1	3.22	119.61	112.07
12	C	701	HEM	CMD-C2D-C3D	3.25	128.71	114.35
12	C	702	HEM	C3B-CAB-CBB	3.27	129.47	124.46
17	D	714	3PH	O13-P-O11	3.36	116.24	106.56
17	A	713	3PH	O13-P-O11	3.42	116.41	106.56
12	C	702	HEM	C3C-CAC-CBC	3.44	129.72	124.46
12	D	703	HEM	CAD-C3D-C4D	3.72	125.59	112.47
12	D	703	HEM	CMC-C2C-C3C	3.75	125.89	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	713	3PH	O11-P-O12	3.77	116.75	107.14
12	D	703	HEM	CMB-C2B-C3B	3.77	125.95	116.53
15	C	706	UQ6	C11-C12-C13	3.82	121.69	111.69
12	C	701	HEM	CAD-C3D-C4D	4.20	127.28	112.47
12	C	702	HEM	CAD-C3D-C2D	4.26	125.48	113.22
15	C	706	UQ6	C21-C19-C18	4.29	129.18	121.05
12	C	702	HEM	CAD-C3D-C4D	4.31	127.66	112.47
12	C	701	HEM	CAD-C3D-C2D	4.35	125.71	113.22
15	C	706	UQ6	C4M-O4-C4	4.75	127.30	114.82
12	C	702	HEM	CMB-C2B-C3B	4.98	128.97	116.53
12	D	703	HEM	CAD-C3D-C2D	5.00	127.60	113.22
12	C	702	HEM	CMC-C2C-C3C	5.31	129.79	116.53
12	C	701	HEM	CMB-C2B-C3B	5.57	130.43	116.53
15	C	706	UQ6	C17-C18-C19	5.90	140.59	127.76
15	C	706	UQ6	C3M-O3-C3	8.02	135.91	114.82

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	D	731	CDL	CA4-OA6-CA5-OA7
20	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
17	A	713	3PH	4	0
19	A	721	UMQ	2	0
12	C	702	HEM	1	0
14	C	705	DBT	1	0
15	C	706	UQ6	8	0
16	C	710	3PE	3	0
17	D	714	3PH	3	0
18	D	715	PC1	3	0
20	D	731	CDL	5	0
13	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 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.