

# wwPDB X-ray Structure Validation Summary Report (i)

#### Aug 8, 2023 – 09:14 PM EDT

PDB ID : 1P84

Title: HDBT inhibited Yeast Cytochrome bc1 Complex

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Deposited on : 2003-05-06

Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : NOT EXECUTED

EDS : NOT EXECUTED

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

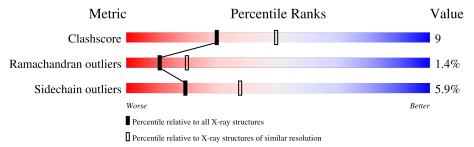
Validation Pipeline (wwPDB-VP) : 2.35

## 1 Overall quality at a glance (i)

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.

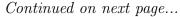


Metric	Whole archive	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain		
1	A	431	76%	22%	•
2	В	352	63% 35%		<u> </u>
3	С	385	85%	14%	
4	D	246	83%	16%	<u>.</u>
5	E	185	82%	17%	<u>.</u>
6	F	74	78%	20%	
7	G	125	90%	10%	
8	Н	93	85%	13%	•





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Mol	Chain	Length	Quality of chain			
9	I	55	85%	-	11%	•
10	J	127	69%	26%		5%
11	K	107	60%	35%		6%



# 2 Entry composition (i)

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

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					AltConf	Trace
2	В	352	Total 2735	C 1747	N 453	O 534	S	0	0	0

• Molecule 3 is a protein called cytochrome b.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	122	THR	ILE	conflict	UNP P00163

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

Mol	Chain	Residues		Atoms					AltConf	Trace
1	D	246	Total	С	N	О	S	0	0	0
4	D	240	1941	1237	334	361	9		U	U

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



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

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

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

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

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

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

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

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

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

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

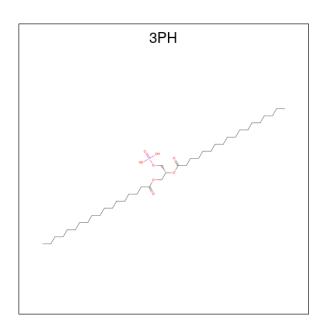
Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
10	J	127	Total 1015	C 644	N 167	O 201	S 3	0	0	0

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

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

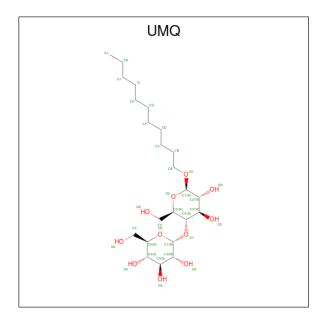
• Molecule 12 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: C<sub>39</sub>H<sub>77</sub>O<sub>8</sub>P).





Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
12	A	1	Total 40				0	0
19	D	1	Total				0	0
12	Ъ	1	38	29	8	1	0	0

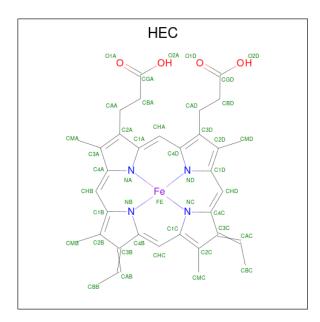
 $\bullet$  Molecule 13 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula:  $\mathrm{C}_{23}\mathrm{H}_{44}\mathrm{O}_{11}).$ 



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

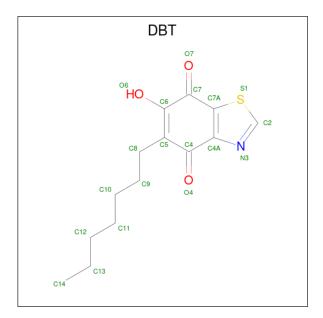
 $\bullet$  Molecule 14 is HEME C (three-letter code: HEC) (formula:  $\rm C_{34}H_{34}FeN_4O_4).$ 





Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf
14	С	1	Total	С	Fe	N	О	0	0
14		1	43	34	1	4	4		0
14	C	1	Total	С	Fe	N	О	0	0
14		1	43	34	1	4	4		0
14	D	1	Total	С	Fe	N	О	0	0
14	D	1	43	34	1	4	4	0	U

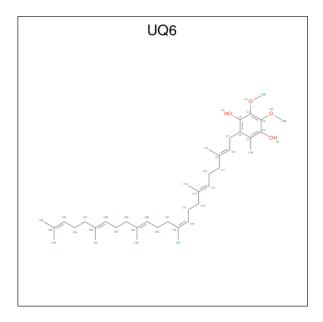
 $\bullet$  Molecule 15 is 5-HEPTYL-6-HYDROXY-1,3-BENZOTHIAZOLE-4,7-DIONE (three-letter code: DBT) (formula: C14H17NO3S).





$\mathbf{Mol}$	Chain	Residues		Ato	$\mathbf{m}\mathbf{s}$		ZeroOcc	AltConf	
15	С	1	Total	С	N	О	S	0	0
19		1	19	14	1	3	1	0	

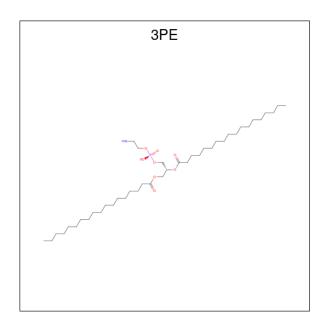
• Molecule 16 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEX AENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (three-letter code: UQ6) (formula:  $C_{39}H_{60}O_4$ ).



Mol	Chain	Residues	Ato	oms		ZeroOcc	AltConf
16	С	1	Total 43	C 39	O 4	0	0

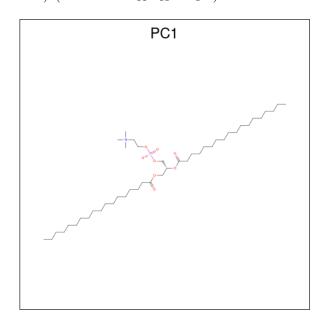
• Molecule 17 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).





Mo	Chai	in	Residues		Ato	oms			ZeroOcc	AltConf	
17	C		1	Total	С	N	О	Р	0	0	
11			1	47	37	1	8	1	U	U	
17	C		1	Total	С	N	О	Р	0	0	
11				40	30	1	8	1	U	U	

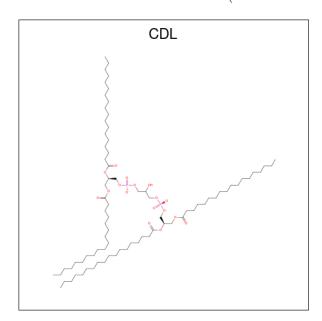
• Molecule 18 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula:  $C_{44}H_{88}NO_8P$ ).



Mol	Chain	Residues		Ato	oms		ZeroOcc	AltConf	
18	D	1	Total		N	O	Р	0	0
		_	38	28	1	8	1		

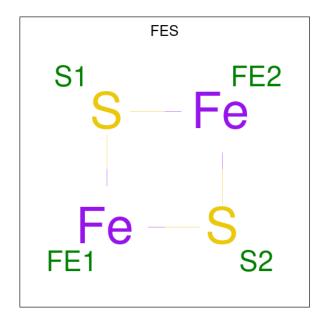


 $\bullet$  Molecule 19 is CARDIOLIPIN (three-letter code: CDL) (formula:  $\mathrm{C_{81}H_{156}O_{17}P_2}).$ 



Mol	Chain	Residues	A	Aton	ns	ZeroOcc	AltConf
19	D	1	Total 76		O 17	0	0

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



Mol	Chain	Residues	Ato	oms		ZeroOcc	AltConf
20	Е	1	Total 4	Fe 2	S 2	0	0

• Molecule 21 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	55	Total O 55 55	0	0
21	В	11	Total O 11 11	0	0
21	С	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	Н	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	К	2	Total O 2 2	0	0

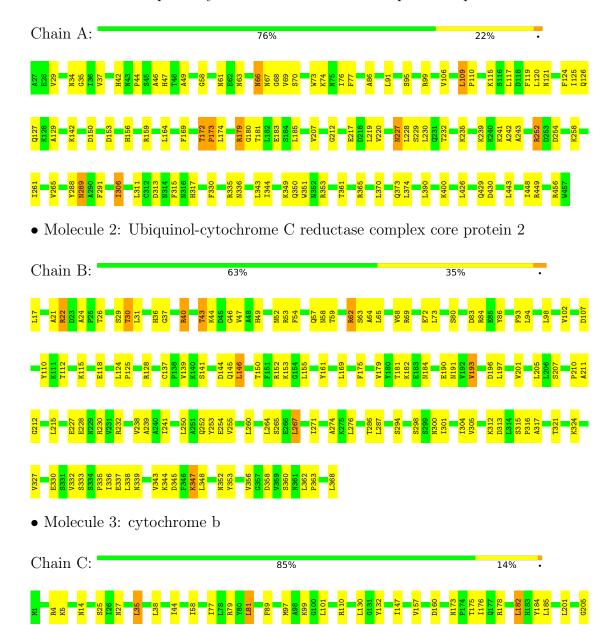


# 3 Residue-property plots (i)

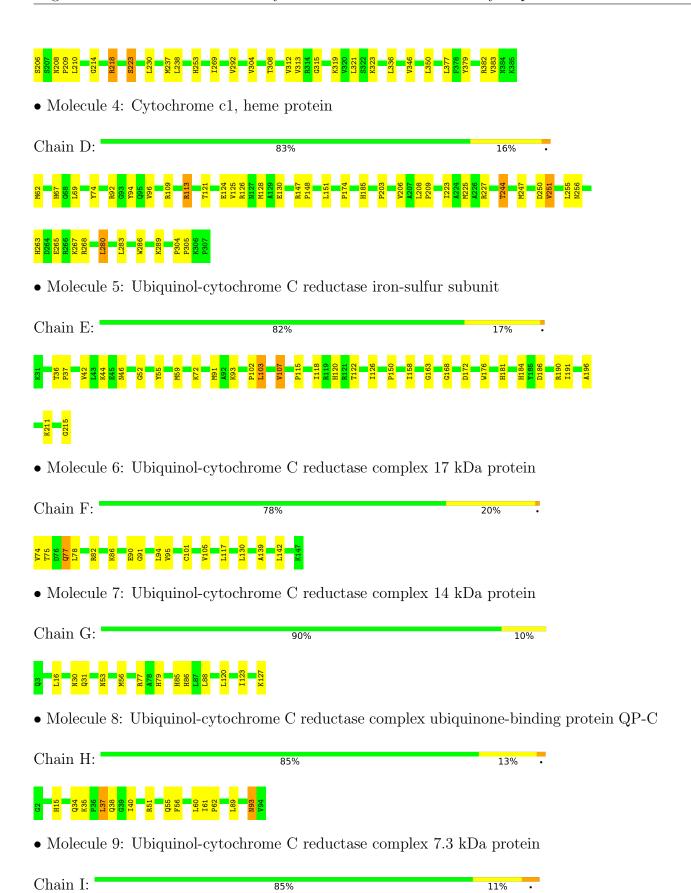
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



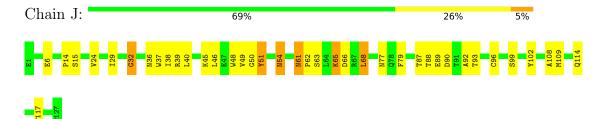




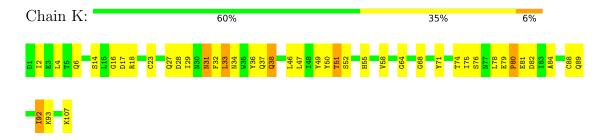




• Molecule 10: Heavy Chain (Vh) Of Fv-Fragment



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





# 4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	C 1 2 1	Depositor	
Cell constants	215.00Å 165.09Å 147.53Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $117.33^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	25.00 - 2.50	Depositor	
% Data completeness	92.5 (25.00-2.50)	Depositor	
(in resolution range)	32.9 (29.00 2.90)		
$R_{merge}$	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 (i)

### 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: UMQ, 3PE, PC1, CDL, DBT, 3PH, HEC, UQ6, FES

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		
MIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.36	0/3405	0.59	0/4614	
2	В	0.33	0/2781	0.59	0/3764	
3	С	0.45	0/3191	0.64	1/4353~(0.0%)	
4	D	0.37	0/2002	0.60	0/2726	
5	Е	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	Н	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 maintenain 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	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
10	J	32	GLY	N-CA-C	6.55	129.48	113.10
3	С	346	VAL	N-CA-C	5.96	127.08	111.00
5	Е	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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

2	B 27 C 30 D 19 E 14 F 62 G 10 H 77 I 44 J 10 K 84 A 4	89 41 11 24 12 73 49 15	0 0 0 0 0 0 0 0	3321 2774 3125 1862 1386 581 1026 736 445	70 83 34 26 24 11 9 12 6	0 0 0 0 0 0 0
3	C 30 D 19 E 144 F 62 G 10 H 77 I 44 J 10 K 84 A 4	89 41 11 24 12 73 49 15	0 0 0 0 0 0 0	3125 1862 1386 581 1026 736 445	34 26 24 11 9 12	0 0 0 0 0
4 I I 5 I I I I I I I I I I I I I I I I	D 19 E 14 F 62 G 10 H 77 I 44 J 10 K 84 A 4	41 11 24 12 73 49 15	0 0 0 0 0 0	1862 1386 581 1026 736 445	26 24 11 9 12	0 0 0 0
5 I G G G G G G G G G G G G G G G G G G	E 14 F 62 G 10 H 77 I 44 J 10 K 84 A 4	11 24 12 73 49 15	0 0 0 0 0	1386 581 1026 736 445	24 11 9 12	0 0 0 0
6	F 62 G 10 H 77 I 44 J 10 K 84 A 4	24 12 73 49 15	0 0 0 0	581 1026 736 445	11 9 12	0 0 0
7	G 10 H 77 I 44 J 10 K 84 A 4	12 73 49 15 12	0 0 0 0	1026 736 445	9 12	0
8	H 77 I 44 J 10 K 84 A 4	73 49 15 42	0 0 0	736 445	12	0
9 10 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	I 44 J 10 K 84 A 4	19 15 12	0	445		
10	J 10 K 84 A 4	15 12	0		6	
11 II I	K 84 A 4	12		0 = 0		0
12 I 12 I 13 I 14 C 14 I 15 C	A 4			959	30	0
12 I 13 A 14 C 14 I 15 C			0	820	25	0
13 A 14 C 14 I 15 C 16 C	D 3	0	0	53	4	0
14 C 14 I 15 C 16 C		8	0	49	3	0
14 I 15 C 16 C		4	0	44	2	0
15 (C) 16 (C)	C 8	6	0	64	3	0
16		3	0	30	1	0
		9	0	17	1	0
	C 4	3	0	58	8	0
17 (	C 8	7	0	128	3	0
18 I	D 3	8	0	50	3	0
	D 7	6	0	99	5	0
20 I		1	0	0	1	0
21 A	A 5	5	0	0	1	0
		1	0	0	0	0
21 (	C 1	10	0	0	5	0
21 I	D 6	2	0	0	0	0
21 I	E 2	5	0	0	0	0
		1	0	0	1	0
	G 3	2	0	0	1	0
21 I		0	0	0	1	0
21	H 2	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	17627	331	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.

The worst 5 of 331 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

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%)	13 24
2	В	350/352~(99%)	304 (87%)	39 (11%)	7 (2%)	7 12
3	С	383/385 (100%)	368 (96%)	14 (4%)	1 (0%)	41 61
4	D	244/246 (99%)	233 (96%)	11 (4%)	0	100 100
5	E	183/185 (99%)	168 (92%)	12 (7%)	3 (2%)	9 17
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	Н	91/93 (98%)	78 (86%)	9 (10%)	4 (4%)	2 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
9	I	53/55~(96%)	49 (92%)	2 (4%)	2 (4%)	3	4
10	J	125/127 (98%)	114 (91%)	8 (6%)	3 (2%)	6	9
11	K	105/107 (98%)	88 (84%)	11 (10%)	6 (6%)	1	1
All	All	2158/2180 (99%)	1983 (92%)	144 (7%)	31 (1%)	11	20

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	152	ARG
2	В	335	PRO
3	С	223	SER
8	Н	93	ASN
11	K	80	PRO

#### 5.3.2 Protein sidechains (i)

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	Perc	entiles
1	A	$370/370\ (100\%)$	343 (93%)	27 (7%)	14	27
2	В	$301/301 \; (100\%)$	277 (92%)	24 (8%)	12	23
3	C	$338/338 \ (100\%)$	316 (94%)	22 (6%)	17	33
4	D	$204/204\ (100\%)$	196 (96%)	8 (4%)	32	57
5	E	$151/151\ (100\%)$	148 (98%)	3 (2%)	55	79
6	F	$67/67 \; (100\%)$	63 (94%)	4 (6%)	19	37
7	G	$109/109\ (100\%)$	105 (96%)	4 (4%)	34	60
8	Н	77/77~(100%)	77 (100%)	0	100	100
9	I	45/45~(100%)	42 (93%)	3 (7%)	16	31
10	J	$112/112 \ (100\%)$	104 (93%)	8 (7%)	14	28
11	K	93/93 (100%)	85 (91%)	8 (9%)	10	20
All	All	1867/1867 (100%)	1756 (94%)	111 (6%)	19	37



5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	С	99	LYS
11	K	107	LYS
3	С	377	LEU
11	K	93	LYS
10	J	66	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
10	J	59	ASN
10	J	77	ASN
11	K	91	HIS
2	В	49	HIS
1	A	438	GLN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

#### 5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

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	В	ond leng	$_{ m gths}$	Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	3PH	A	713	-	39,39,47	1.14	4 (10%)	43,44,52	1.60	5 (11%)
14	HEC	D	703	4	32,50,50	1.60	2 (6%)	24,82,82	1.08	1 (4%)
19	CDL	D	731	-	75,75,99	1.63	13 (17%)	81,87,111	1.47	12 (14%)
17	3PE	С	711	-	39,39,50	0.83	1 (2%)	42,44,55	1.03	2 (4%)
14	HEC	С	701	3	32,50,50	1.56	5 (15%)	24,82,82	1.57	4 (16%)
20	FES	Е	704	5	0,4,4	-	-	-		
14	HEC	С	702	3	32,50,50	1.45	3 (9%)	24,82,82	1.59	6 (25%)
15	DBT	С	705	-	15,20,20	1.30	2 (13%)	16,27,27	1.29	2 (12%)
13	UMQ	A	721	-	35,35,35	1.04	2 (5%)	46,46,46	1.73	8 (17%)
16	UQ6	С	706	-	43,43,43	3.20	18 (41%)	51,55,55	2.19	14 (27%)
12	3PH	D	714	-	37,37,47	1.04	1 (2%)	41,42,52	1.58	9 (21%)
17	3PE	С	710	-	46,46,50	1.15	6 (13%)	49,51,55	1.27	3 (6%)
18	PC1	D	715	-	37,37,53	2.03	9 (24%)	43,45,61	1.52	7 (16%)

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	-	-	19/41/41/49	-
14	HEC	D	703	4	-	2/10/54/54	-
19	CDL	D	731	-	-	40/86/86/110	-
17	3PE	С	711	-	-	15/43/43/54	-
14	HEC	С	701	3	-	4/10/54/54	-
20	FES	E	704	5	-	-	0/1/1/1
14	HEC	С	702	3	-	4/10/54/54	-
15	DBT	С	705	-	-	2/7/27/27	0/2/2/2
13	UMQ	A	721	-	-	6/20/60/60	0/2/2/2
16	UQ6	С	706	-	-	18/39/39/39	0/1/1/1
12	3PH	D	714	-	-	8/39/39/49	-
17	3PE	С	710	-	-	20/50/50/54	-
18	PC1	D	715	-	-	19/41/41/57	-

The worst 5 of 66 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(A)
16	С	706	UQ6	C7-C6	10.82	1.63	1.51
16	С	706	UQ6	C5-C6	7.70	1.51	1.40
16	С	706	UQ6	C5-C4	7.30	1.51	1.39
18	D	715	PC1	O21-C21	7.24	1.54	1.34
18	D	715	PC1	O31-C31	6.21	1.51	1.33

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
13	A	721	UMQ	CA-O1'-C1'	-8.02	100.54	113.84
16	С	706	UQ6	C3M-O3-C3	7.71	135.91	114.78
19	D	731	CDL	CB4-OB6-CB5	-6.23	102.45	117.79
16	С	706	UQ6	C17-C18-C19	5.37	140.59	127.66
12	A	713	3PH	P-O11-C1	5.34	133.00	118.30

There are no chirality outliers.

5 of 157 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	С	706	UQ6	C18-C19-C21-C22
16	С	706	UQ6	C20-C19-C21-C22
16	С	706	UQ6	C19-C21-C22-C23
17	С	710	3PE	O13-C11-C12-N
17	С	711	3PE	C1-O11-P-O12

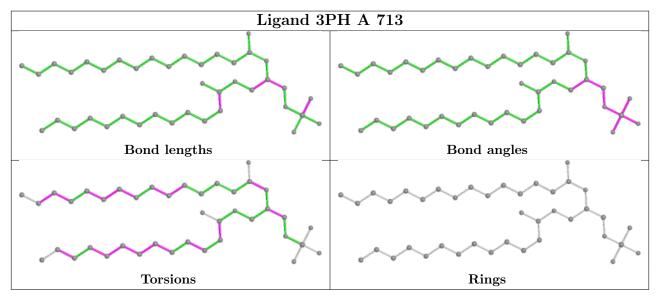
There are no ring outliers.

12 monomers are involved in 33 short contacts:

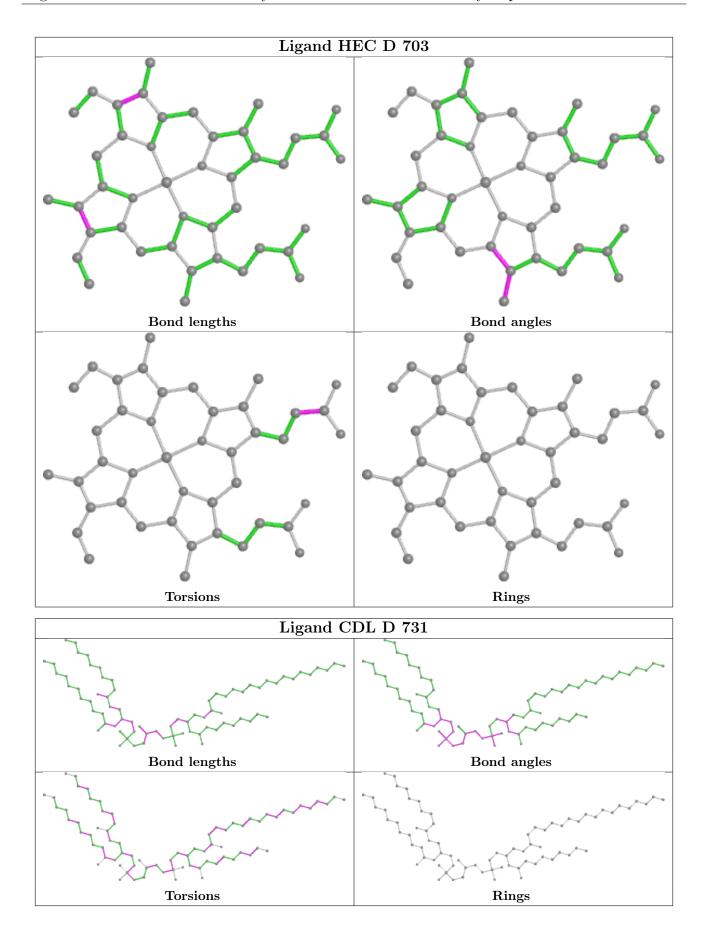
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	713	3PH	4	0
14	D	703	HEC	1	0
19	D	731	CDL	5	0
14	С	701	HEC	2	0
20	Е	704	FES	1	0
14	С	702	HEC	1	0
15	С	705	DBT	1	0
13	A	721	UMQ	2	0
16	С	706	UQ6	8	0
12	D	714	3PH	3	0
17	С	710	3PE	3	0
18	D	715	PC1	3	0



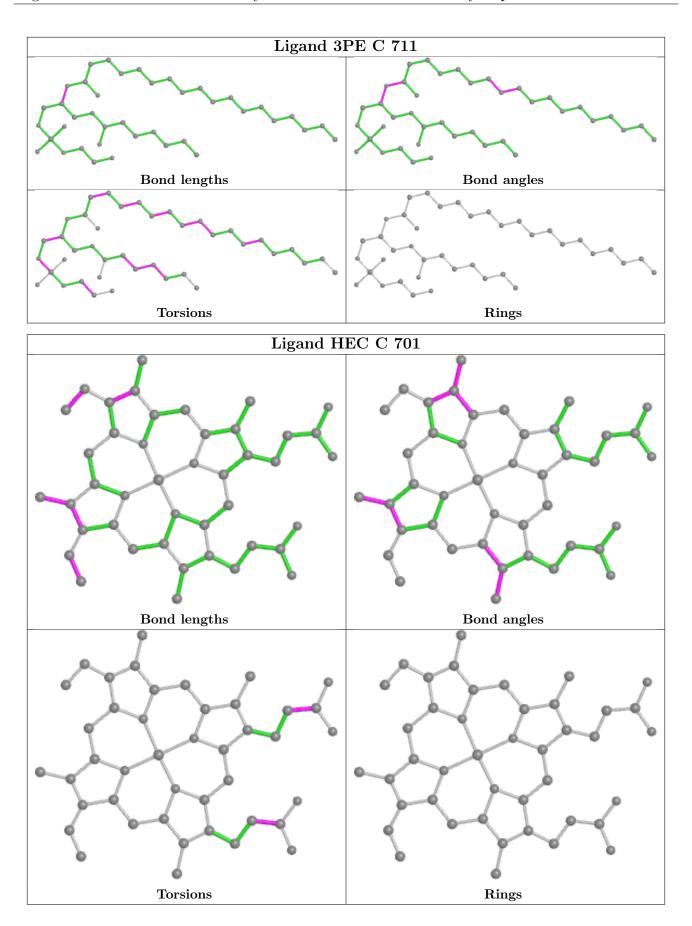
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



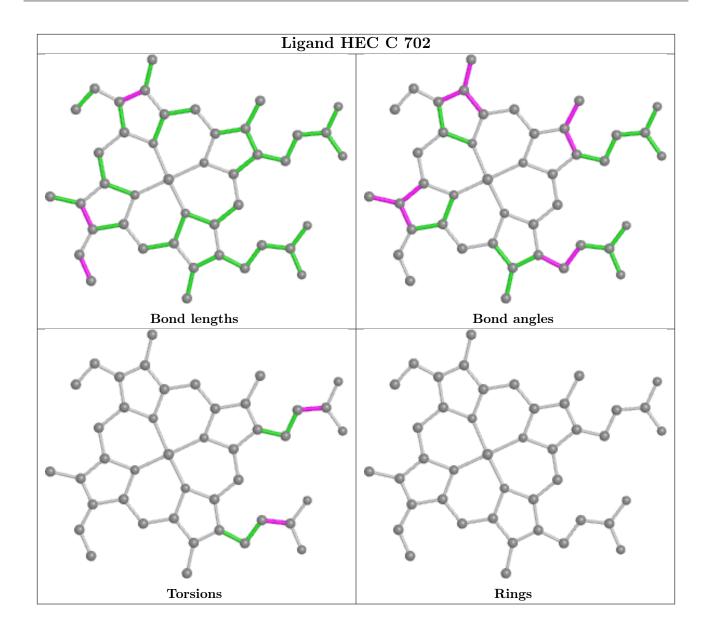




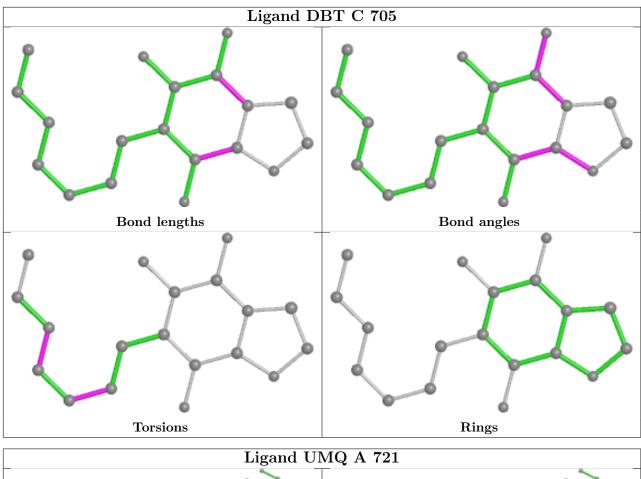


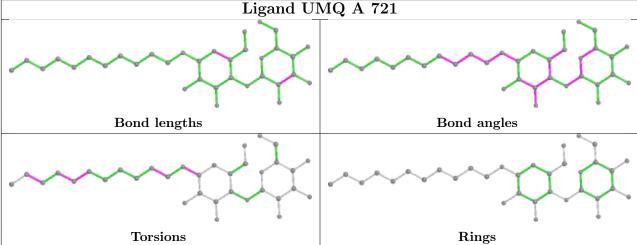




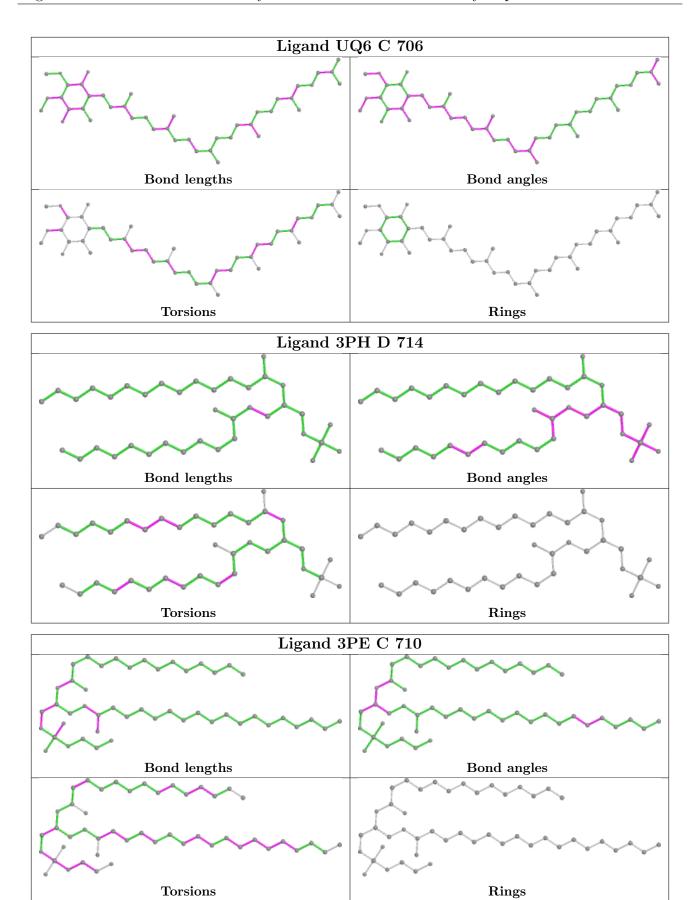




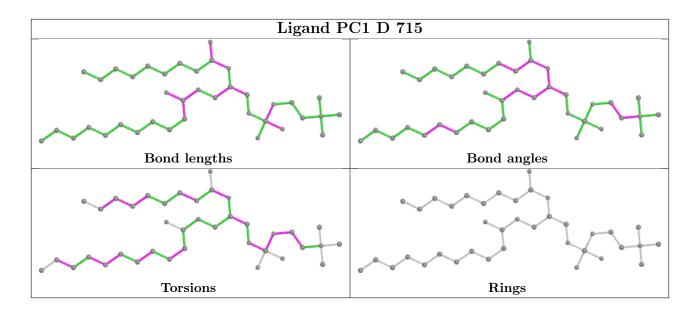












# 5.7 Other polymers (i)

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 (i)

#### 6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

