Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 09:22 AM EDT

PDB ID	:	1SQQ
Title	:	Crystal Structure Analysis of Bovine Bc1 with Methoxy Acrylate Stilbene (MOAS)
Authors	:	Esser, L.; Quinn, B.; Li, Y.F.; Zhang, M.; Elberry, M.; Yu, L.; Yu, C.A.; Xia, D.
Deposited on	:	2004-03-19
Resolution	:	3.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

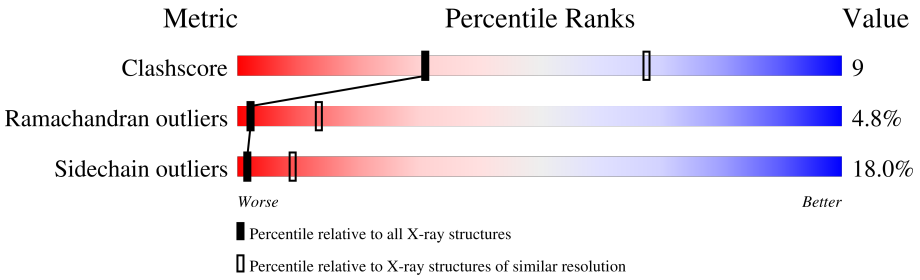
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	446	64% 26% 8% •
2	B	439	66% 23% 6% • •
3	C	379	59% 34% 5% •
4	D	241	50% 37% 10% •
5	E	196	71% 23% • •
6	F	110	58% 30% 6% • 5%
7	G	81	57% 28% 6% • 7%
8	H	78	35% 35% 17% • 10%

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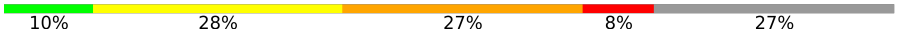
Mol	Chain	Length	Quality of chain
9	I	78	
10	J	62	
11	K	56	

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 16887 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial precursor.

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

- Molecule 2 is a protein called Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial precursor.

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

- Molecule 3 is a protein called Cytochrome b.

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

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

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

- Molecule 5 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial precursor (EC 1.10.2.2) (Rieske iron-sulfur protein) (RISP) [Contains: Ubiquinol-cytochrome c reductase 8 kDa protein (Complex III subunit IX)].

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

- Molecule 6 is a protein called Ubiquinol-cytochrome c reductase complex 14 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	105	Total	C	N	O	S	0	0	0
			911	576	165	168	2			

- Molecule 7 is a protein called Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	70	Total	C	N	O	S	0	0	0
			575	347	102	121	5			

- Molecule 9 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial precursor (EC 1.10.2.2) (Rieske iron-sulfur protein) (RISP) [Contains: Ubiquinol-cytochrome c reductase 8 kDa protein (Complex III subunit IX)].

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

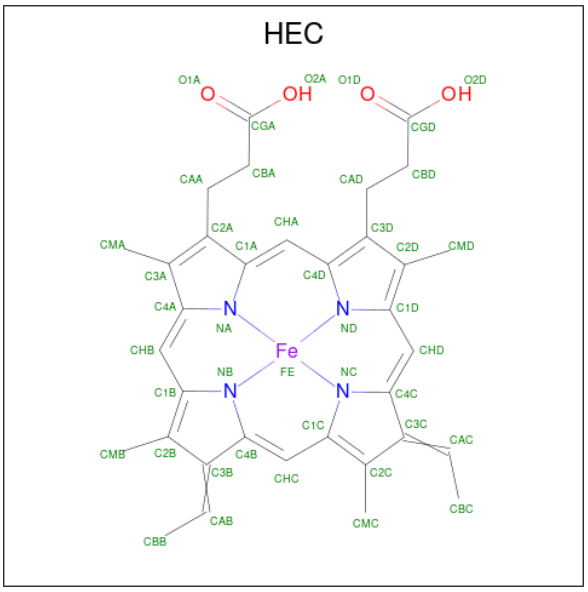
- Molecule 10 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	59	Total	C	N	O	0	0	0
			490	321	85	84			

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

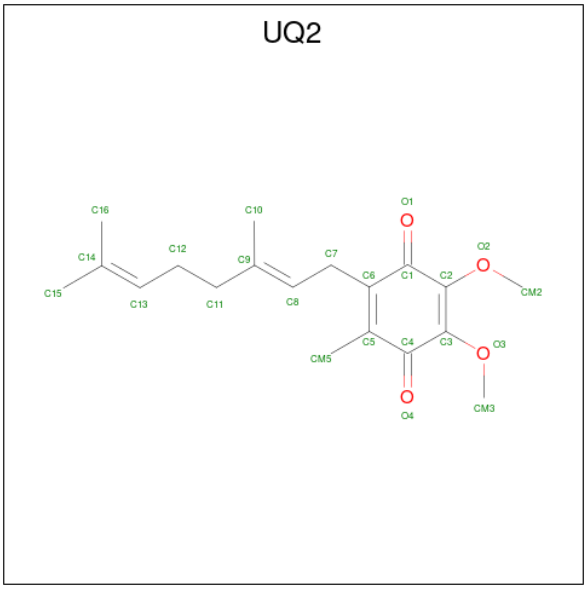
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	54	Total	C	N	O	S	0	0	0
			447	299	80	67	1			

- Molecule 12 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



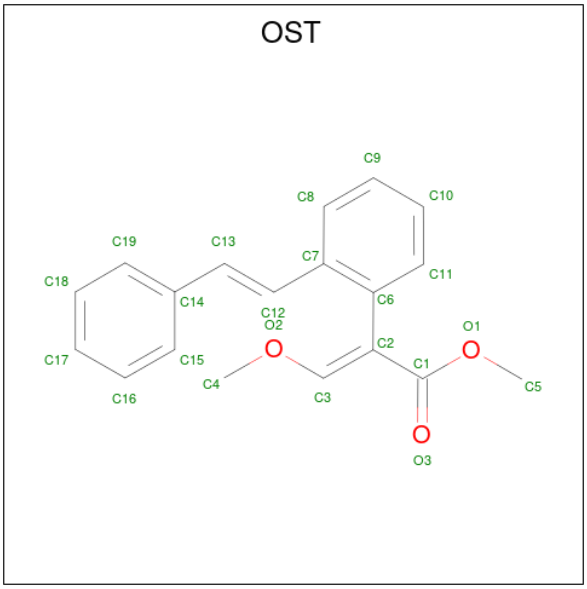
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 13 is UBIQUINONE-2 (three-letter code: UQ2) (formula: $C_{19}H_{26}O_4$).



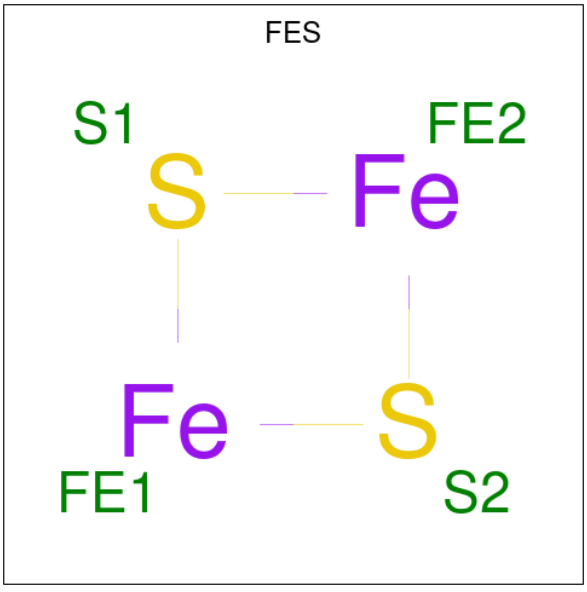
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	O	0	0
			23	19	4		

- Molecule 14 is METHYL (2Z)-3-METHOXY-2-{2-[(E)-2-PHENYLVINYL]PHENYL}ACRYLATE (three-letter code: OST) (formula: $C_{19}H_{18}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	C	1	Total C O 22 19 3	0	0

- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 16 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	31	Total O 31 31	0	0
16	B	78	Total O 78 78	0	0
16	C	21	Total O 21 21	0	0
16	D	5	Total O 5 5	0	0
16	E	1	Total O 1 1	0	0
16	F	25	Total O 25 25	0	0
16	G	12	Total O 12 12	0	0
16	H	2	Total O 2 2	0	0
16	I	4	Total O 4 4	0	0
16	J	1	Total O 1 1	0	0
16	K	2	Total O 2 2	0	0

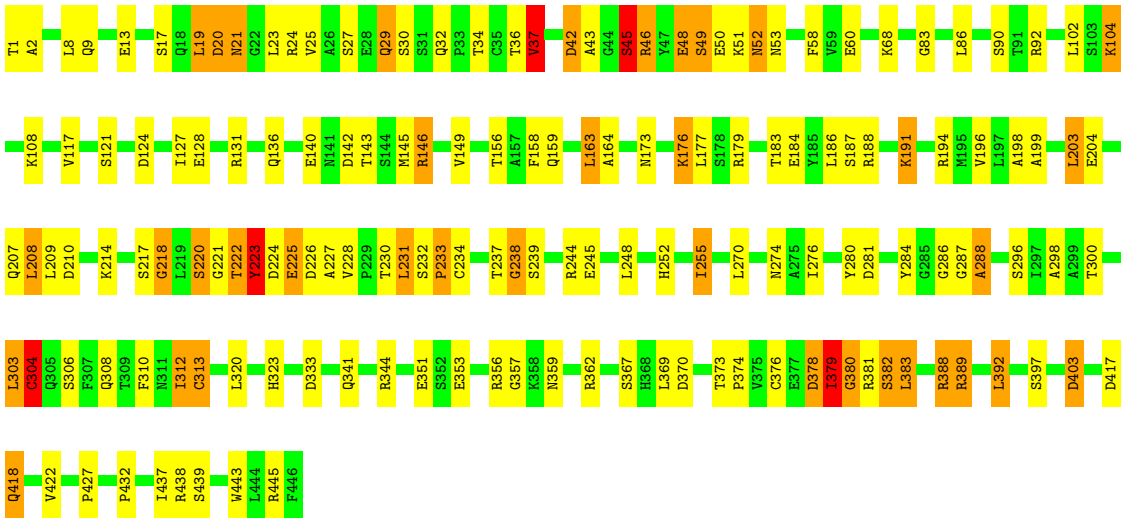
3 Residue-property plots (i)

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.

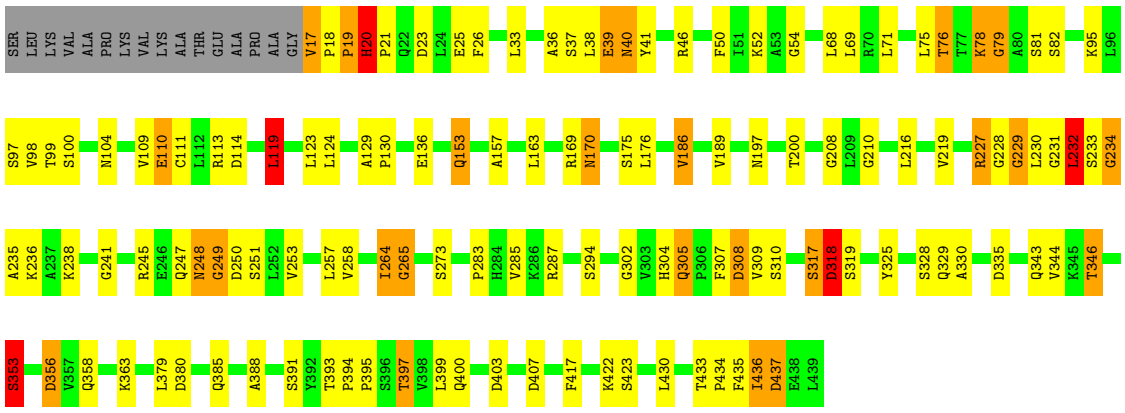
• Molecule 1: Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial precursor

Chain A:



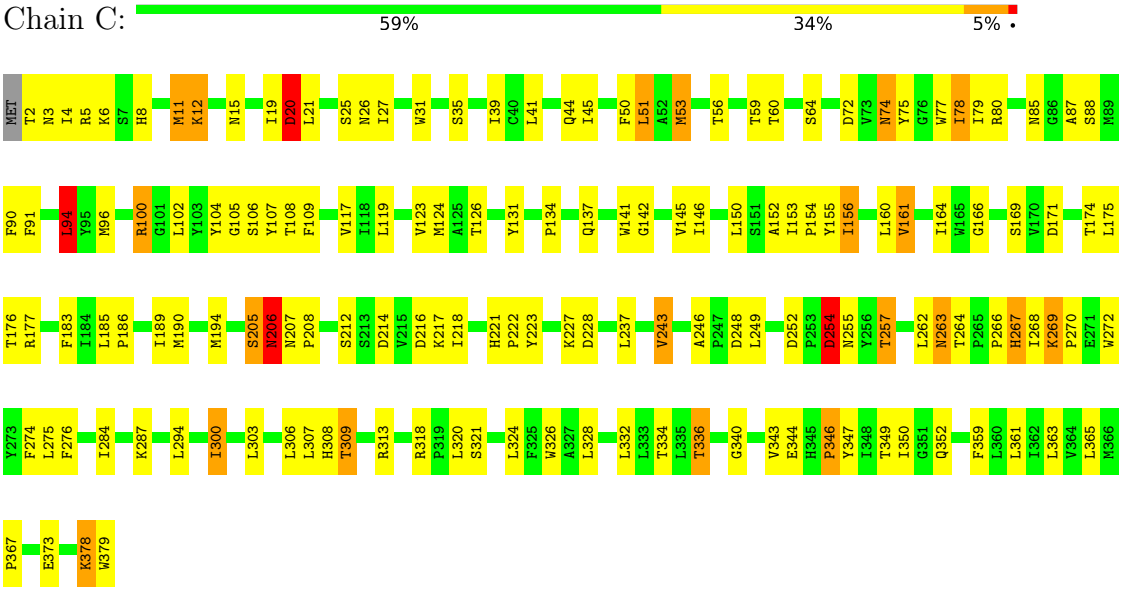
• Molecule 2: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial precursor

Chain B:



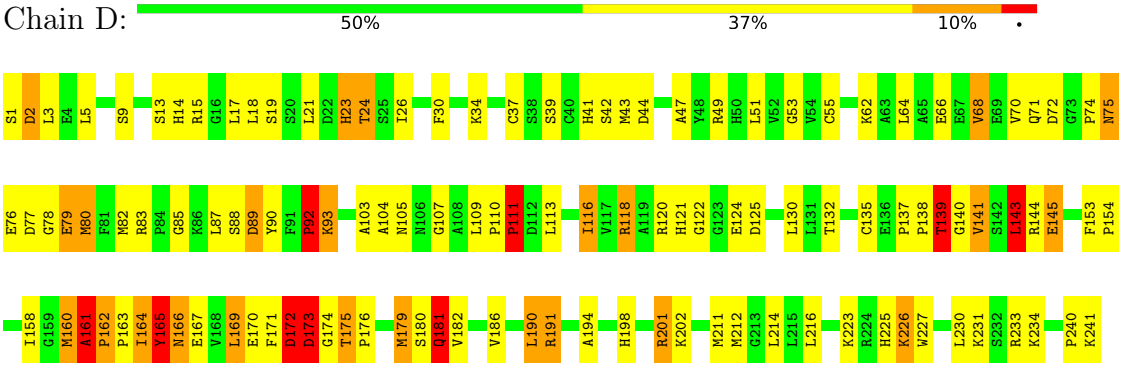
• Molecule 3: Cytochrome b

Chain C:



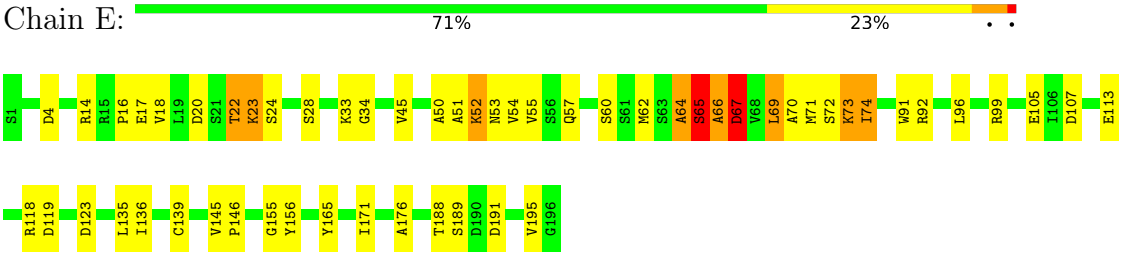
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D:



• Molecule 5: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial precursor (EC 1.10.2.2) (Rieske iron-sulfur protein) (RISP) [Contains: Ubiquinol-cytochrome c reductase 8 kDa protein (Complex III subunit IX)]

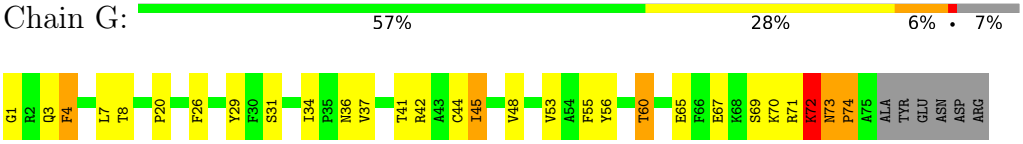
Chain E:



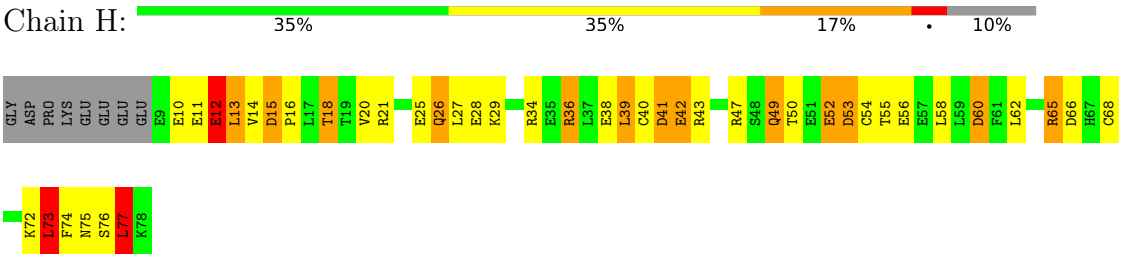
• Molecule 6: Ubiquinol-cytochrome c reductase complex 14 kDa protein

Chain F:

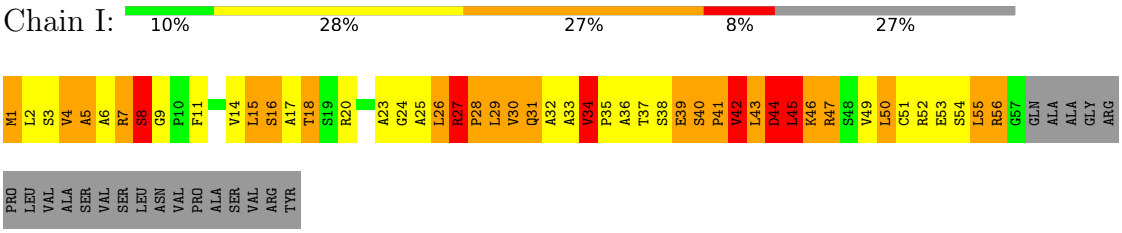
• Molecule 7: Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C



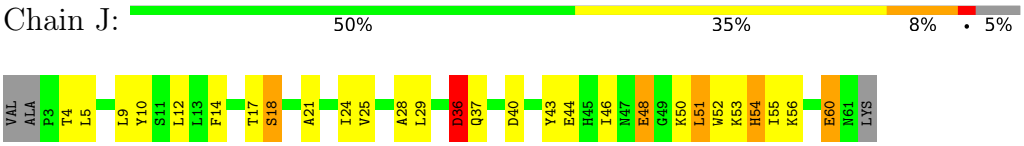
• Molecule 8: Ubiquinol-cytochrome c reductase complex 11 kDa protein



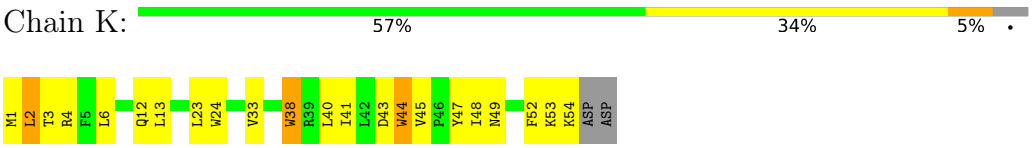
• Molecule 9: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial precursor (EC 1.10.2.2) (Rieske iron-sulfur protein) (RISP) [Contains: Ubiquinol-cytochrome c reductase 8 kDa protein (Complex III subunit IX)]



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



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



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	153.68Å 153.68Å 598.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00	Depositor
% Data completeness (in resolution range)	96.8 (50.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.228 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16887	wwPDB-VP
Average B, all atoms (Å^2)	26.0	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: UQ2, FES, OST, HEC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.98	2/3531 (0.1%)	0.86	9/4792 (0.2%)
2	B	1.09	2/3232 (0.1%)	0.91	11/4386 (0.3%)
3	C	1.07	1/3100 (0.0%)	0.87	6/4242 (0.1%)
4	D	0.99	0/1977	0.86	8/2684 (0.3%)
5	E	0.65	0/1553	0.81	6/2100 (0.3%)
6	F	1.13	1/930 (0.1%)	0.97	5/1246 (0.4%)
7	G	1.20	2/649 (0.3%)	0.86	0/878
8	H	0.95	0/580	0.96	4/777 (0.5%)
9	I	1.47	1/411 (0.2%)	1.23	3/558 (0.5%)
10	J	1.15	0/503	0.86	2/678 (0.3%)
11	K	1.14	0/463	0.86	1/632 (0.2%)
All	All	1.04	9/16929 (0.1%)	0.89	55/22973 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	28
2	B	0	33
3	C	0	20
4	D	0	50
6	F	0	4
7	G	0	4
8	H	0	15
9	I	0	33
10	J	0	8
11	K	0	8
All	All	0	203

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	288	ALA	CA-CB	-5.95	1.40	1.52
3	C	91	PHE	CE2-CZ	5.65	1.48	1.37
2	B	26	PHE	CE2-CZ	5.64	1.48	1.37
7	G	55	PHE	CD2-CE2	5.54	1.50	1.39
9	I	42	VAL	CA-CB	5.42	1.66	1.54
6	F	55	TYR	CE1-CZ	5.27	1.45	1.38
2	B	50	PHE	CE1-CZ	5.19	1.47	1.37
1	A	304	CYS	CB-SG	-5.17	1.73	1.81
7	G	55	PHE	CD1-CE1	5.08	1.49	1.39

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	57	ASP	CB-CG-OD2	8.34	125.80	118.30
3	C	248	ASP	CB-CG-OD2	7.93	125.44	118.30
9	I	45	LEU	CA-CB-CG	7.19	131.83	115.30
1	A	333	ASP	CB-CG-OD2	7.06	124.65	118.30
2	B	318	ASP	CB-CG-OD2	7.04	124.63	118.30
9	I	44	ASP	CB-CG-OD2	6.98	124.58	118.30
2	B	114	ASP	CB-CG-OD2	6.93	124.54	118.30
2	B	23	ASP	CB-CG-OD2	6.84	124.46	118.30
8	H	15	ASP	CB-CG-OD2	6.83	124.45	118.30
6	F	41	ASP	CB-CG-OD2	6.67	124.30	118.30
3	C	20	ASP	CB-CG-OD2	6.58	124.22	118.30
3	C	214	ASP	CB-CG-OD2	6.52	124.17	118.30
1	A	142	ASP	CB-CG-OD2	6.52	124.17	118.30
5	E	4	ASP	CB-CG-OD2	6.36	124.02	118.30
6	F	35	ASP	CB-CG-OD2	6.23	123.91	118.30
1	A	210	ASP	CB-CG-OD2	6.22	123.89	118.30
11	K	43	ASP	CB-CG-OD2	6.20	123.88	118.30
2	B	356	ASP	CB-CG-OD2	6.17	123.85	118.30
9	I	43	LEU	CA-CB-CG	6.11	129.36	115.30
4	D	125	ASP	CB-CG-OD2	6.02	123.72	118.30
4	D	44	ASP	CB-CG-OD2	5.99	123.69	118.30
1	A	42	ASP	CB-CG-OD2	5.93	123.64	118.30
2	B	403	ASP	CB-CG-OD2	5.91	123.62	118.30
4	D	173	ASP	CB-CG-OD2	5.84	123.55	118.30
8	H	60	ASP	CB-CG-OD2	5.82	123.54	118.30
5	E	67	ASP	CB-CG-OD2	5.79	123.51	118.30
2	B	335	ASP	CB-CG-OD2	5.79	123.51	118.30
4	D	2	ASP	CB-CG-OD2	5.73	123.46	118.30
1	A	403	ASP	CB-CG-OD2	5.73	123.45	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	94	LEU	CA-CB-CG	5.68	128.37	115.30
6	F	56	ASP	CB-CG-OD2	5.66	123.39	118.30
4	D	172	ASP	CB-CG-OD2	5.58	123.32	118.30
2	B	232	LEU	CA-CB-CG	5.54	128.05	115.30
10	J	40	ASP	CB-CG-OD2	5.52	123.26	118.30
5	E	123	ASP	CB-CG-OD2	5.50	123.25	118.30
2	B	407	ASP	CB-CG-OD2	5.49	123.24	118.30
2	B	380	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	20	ASP	CB-CG-OD2	5.47	123.22	118.30
4	D	77	ASP	CB-CG-OD2	5.38	123.15	118.30
8	H	73	LEU	CA-CB-CG	5.34	127.58	115.30
1	A	124	ASP	CB-CG-OD2	5.29	123.06	118.30
5	E	191	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	370	ASP	CB-CG-OD2	5.23	123.01	118.30
4	D	89	ASP	CB-CG-OD2	5.23	123.00	118.30
5	E	119	ASP	CB-CG-OD2	5.23	123.00	118.30
4	D	92	PRO	N-CA-C	5.22	125.67	112.10
8	H	66	ASP	CB-CG-OD2	5.17	122.96	118.30
6	F	34	ASP	CB-CG-OD2	5.14	122.92	118.30
5	E	107	ASP	CB-CG-OD2	5.11	122.90	118.30
3	C	252	ASP	CB-CG-OD2	5.11	122.90	118.30
3	C	254	ASP	CB-CG-OD2	5.08	122.87	118.30
2	B	308	ASP	CB-CG-OD2	5.06	122.85	118.30
2	B	119	LEU	CA-CB-CG	-5.06	103.67	115.30
1	A	378	ASP	CB-CG-OD2	5.03	122.83	118.30
10	J	36	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (203) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	191	LYS	Peptide
1	A	20	ASP	Peptide
1	A	218	GLY	Peptide
1	A	220	SER	Peptide
1	A	221	GLY	Peptide
1	A	222	THR	Peptide
1	A	223	TYR	Peptide
1	A	225	GLU	Peptide
1	A	227	ALA	Peptide
1	A	228	VAL	Peptide
1	A	231	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	A	232	SER	Peptide
1	A	234	CYS	Peptide
1	A	238	GLY	Peptide
1	A	27	SER	Peptide
1	A	286	GLY	Peptide
1	A	287	GLY	Peptide
1	A	303	LEU	Peptide
1	A	306	SER	Peptide
1	A	312	ILE	Peptide
1	A	356	ARG	Peptide
1	A	37	VAL	Peptide
1	A	379	ILE	Peptide
1	A	388	ARG	Peptide
1	A	43	ALA	Peptide
1	A	45	SER	Peptide
1	A	49	SER	Peptide
1	A	50	GLU	Peptide
2	B	100	SER	Peptide
2	B	153	GLN	Peptide
2	B	169	ARG	Peptide
2	B	17	VAL	Peptide
2	B	170	ASN	Peptide
2	B	19	PRO	Peptide
2	B	210	GLY	Peptide
2	B	227	ARG	Peptide
2	B	228	GLY	Peptide
2	B	229	GLY	Peptide
2	B	231	GLY	Peptide
2	B	233	SER	Peptide
2	B	234	GLY	Peptide
2	B	235	ALA	Peptide
2	B	248	ASN	Peptide
2	B	249	GLY	Peptide
2	B	251	SER	Peptide
2	B	265	GLY	Peptide
2	B	302	GLY	Peptide
2	B	304	HIS	Peptide
2	B	305	GLN	Peptide
2	B	307	PHE	Peptide
2	B	317	SER	Peptide
2	B	318	ASP	Peptide
2	B	328	SER	Peptide

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Mol	Chain	Res	Type	Group
2	B	353	SER	Peptide
2	B	388	ALA	Peptide
2	B	39	GLU	Peptide
2	B	391	SER	Peptide
2	B	434	PRO	Peptide
2	B	436	ILE	Peptide
2	B	78	LYS	Peptide
2	B	79	GLY	Peptide
3	C	108	THR	Peptide
3	C	11	MET	Peptide
3	C	141	TRP	Peptide
3	C	155	TYR	Peptide
3	C	156	ILE	Peptide
3	C	166	GLY	Peptide
3	C	169	SER	Peptide
3	C	20	ASP	Peptide
3	C	205	SER	Peptide
3	C	221	HIS	Peptide
3	C	25	SER	Peptide
3	C	255	ASN	Peptide
3	C	263	ASN	Peptide
3	C	267	HIS	Peptide
3	C	270	PRO	Peptide
3	C	340	GLY	Peptide
3	C	343	VAL	Peptide
3	C	344	GLU	Peptide
3	C	346	PRO	Peptide
3	C	53	MET	Peptide
4	D	1	SER	Peptide
4	D	103	ALA	Peptide
4	D	104	ALA	Peptide
4	D	105	ASN	Peptide
4	D	107	GLY	Peptide
4	D	109	LEU	Peptide
4	D	111	PRO	Peptide
4	D	122	GLY	Peptide
4	D	135	CYS	Peptide
4	D	137	PRO	Peptide
4	D	138	PRO	Peptide
4	D	139	THR	Peptide
4	D	14	HIS	Peptide
4	D	140	GLY	Peptide

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Mol	Chain	Res	Type	Group
4	D	141	VAL	Peptide
4	D	143	LEU	Peptide
4	D	144	ARG	Peptide
4	D	145	GLU	Peptide
4	D	153	PHE	Peptide
4	D	160	MET	Peptide
4	D	161	ALA	Peptide
4	D	162	PRO	Peptide
4	D	164	ILE	Peptide
4	D	165	TYR	Peptide
4	D	167	GLU	Peptide
4	D	169	LEU	Peptide
4	D	171	PHE	Peptide
4	D	172	ASP	Peptide
4	D	173	ASP	Peptide
4	D	174	GLY	Peptide
4	D	175	THR	Peptide
4	D	176	PRO	Peptide
4	D	18	LEU	Peptide
4	D	181	GLN	Peptide
4	D	23	HIS	Peptide
4	D	240	PRO	Peptide
4	D	51	LEU	Peptide
4	D	53	GLY	Peptide
4	D	68	VAL	Peptide
4	D	70	VAL	Peptide
4	D	74	PRO	Peptide
4	D	75	ASN	Peptide
4	D	76	GLU	Peptide
4	D	78	GLY	Peptide
4	D	79	GLU	Peptide
4	D	85	GLY	Peptide
4	D	87	LEU	Peptide
4	D	88	SER	Peptide
4	D	92	PRO	Peptide
4	D	93	LYS	Peptide
6	F	6	VAL	Peptide
6	F	83	TYR	Peptide
6	F	86	ASP	Peptide
6	F	99	ARG	Mainchain
7	G	1	GLY	Peptide
7	G	70	LYS	Peptide

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Mol	Chain	Res	Type	Group
7	G	72	LYS	Peptide
7	G	74	PRO	Peptide
8	H	11	GLU	Peptide
8	H	12	GLU	Peptide
8	H	13	LEU	Peptide
8	H	25	GLU	Peptide
8	H	26	GLN	Peptide
8	H	27	LEU	Peptide
8	H	28	GLU	Peptide
8	H	41	ASP	Peptide
8	H	49	GLN	Peptide
8	H	50	THR	Peptide
8	H	52	GLU	Peptide
8	H	53	ASP	Peptide
8	H	73	LEU	Peptide
8	H	76	SER	Peptide
8	H	77	LEU	Peptide
9	I	1	MET	Peptide
9	I	16	SER	Peptide
9	I	17	ALA	Peptide
9	I	23	ALA	Peptide
9	I	24	GLY	Peptide
9	I	26	LEU	Peptide
9	I	27	ARG	Peptide
9	I	28	PRO	Peptide
9	I	29	LEU	Peptide
9	I	3	SER	Peptide
9	I	33	ALA	Peptide
9	I	34	VAL	Peptide
9	I	35	PRO	Peptide
9	I	36	ALA	Peptide
9	I	38	SER	Peptide
9	I	39	GLU	Peptide
9	I	4	VAL	Peptide
9	I	40	SER	Peptide
9	I	41	PRO	Peptide
9	I	42	VAL	Peptide,Mainchain
9	I	44	ASP	Peptide
9	I	45	LEU	Peptide
9	I	46	LYS	Peptide
9	I	49	VAL	Peptide
9	I	51	CYS	Peptide

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Mol	Chain	Res	Type	Group
9	I	52	ARG	Peptide
9	I	54	SER	Peptide
9	I	55	LEU	Peptide
9	I	56	ARG	Peptide
9	I	6	ALA	Peptide
9	I	7	ARG	Peptide
9	I	8	SER	Peptide
10	J	17	THR	Peptide
10	J	36	ASP	Peptide
10	J	43	TYR	Peptide
10	J	46	ILE	Peptide
10	J	48	GLU	Peptide
10	J	51	LEU	Peptide
10	J	53	LYS	Peptide
10	J	60	GLU	Peptide
11	K	2	LEU	Peptide
11	K	3	THR	Peptide
11	K	38	TRP	Peptide
11	K	44	TRP	Peptide
11	K	45	VAL	Peptide
11	K	47	TYR	Peptide
11	K	48	ILE	Peptide
11	K	53	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3458	0	3355	67	0
2	B	3172	0	3152	56	0
3	C	3003	0	3065	74	0
4	D	1918	0	1870	32	0
5	E	1519	0	1502	53	0
6	F	911	0	904	15	0
7	G	628	0	636	11	0
8	H	575	0	548	10	0
9	I	406	0	437	29	0
10	J	490	0	489	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	447	0	460	2	0
12	C	86	0	64	12	0
12	D	43	0	32	3	0
13	C	23	0	26	8	0
14	C	22	0	18	4	0
15	E	4	0	0	0	0
16	A	31	0	0	3	0
16	B	78	0	0	2	0
16	C	21	0	0	2	0
16	D	5	0	0	0	0
16	E	1	0	0	0	0
16	F	25	0	0	1	0
16	G	12	0	0	0	0
16	H	2	0	0	0	0
16	I	4	0	0	1	0
16	J	1	0	0	0	0
16	K	2	0	0	0	0
All	All	16887	0	16558	303	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 (303) 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)
3:C:124:MET:SD	3:C:124:MET:CE	2.03	1.44
1:A:237:THR:OG1	5:E:14:ARG:NH2	1.85	1.09
2:B:310:SER:HB3	9:I:28:PRO:HD3	1.41	1.03
1:A:284:TYR:HE1	9:I:20:ARG:HG2	1.34	0.92
4:D:37:CYS:SG	12:D:242:HEC:HAB	2.15	0.86
1:A:308:GLN:HE21	1:A:323:HIS:HD2	1.26	0.82
3:C:35:SER:HB3	13:C:383:UQ2:H5M2	1.61	0.81
7:G:73:ASN:HB3	7:G:74:PRO:HD3	1.63	0.81
3:C:119:LEU:HD22	12:C:382:HEC:HBB3	1.61	0.81
5:E:72:SER:HB3	5:E:92:ARG:HE	1.44	0.80
2:B:76:THR:HG22	2:B:82:SER:H	1.45	0.80
2:B:308:ASP:HB2	9:I:32:ALA:HB2	1.67	0.77
1:A:284:TYR:CE1	9:I:20:ARG:HG2	2.20	0.76
5:E:64:ALA:O	5:E:65:SER:HB2	1.83	0.76
3:C:53:MET:HE1	5:E:62:MET:HG2	1.68	0.75
2:B:247:GLN:HE22	2:B:430:LEU:H	1.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:118:ARG:NH1	5:E:176:ALA:O	2.20	0.72
2:B:325:TYR:HB3	9:I:28:PRO:HD2	1.71	0.71
5:E:156:TYR:HB2	5:E:165:TYR:HB2	1.71	0.71
6:F:84:GLU:O	6:F:85:GLU:HB2	1.90	0.71
6:F:68:LEU:HD23	6:F:71:ARG:HH12	1.56	0.70
9:I:11:PHE:HE2	9:I:25:ALA:H	1.39	0.70
2:B:95:LYS:HA	9:I:18:THR:HG21	1.73	0.69
2:B:157:ALA:HA	9:I:11:PHE:HE1	1.57	0.69
1:A:237:THR:HG23	5:E:14:ARG:HH21	1.56	0.69
3:C:72:ASP:OD2	5:E:67:ASP:OD2	2.10	0.69
7:G:41:THR:O	7:G:45:ILE:HG12	1.91	0.69
10:J:10:TYR:HA	10:J:14:PHE:HB2	1.75	0.68
2:B:76:THR:HB	2:B:81:SER:HA	1.74	0.68
9:I:32:ALA:HB1	16:I:80:HOH:O	1.93	0.68
1:A:45:SER:HA	1:A:48:GLU:HG2	1.74	0.68
3:C:272:TRP:HA	3:C:275:LEU:HG	1.76	0.67
5:E:18:VAL:HG12	5:E:18:VAL:O	1.94	0.67
1:A:237:THR:CG2	5:E:14:ARG:HH21	2.08	0.67
3:C:31:TRP:HA	16:C:1001:HOH:O	1.95	0.67
3:C:53:MET:CE	5:E:62:MET:HG2	2.24	0.66
2:B:283:PRO:HG3	9:I:31:GLN:HG3	1.76	0.66
2:B:153:GLN:NE2	9:I:46:LYS:HG3	2.11	0.66
5:E:139:CYS:SG	5:E:165:TYR:OH	2.52	0.65
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.78	0.65
4:D:118:ARG:HG3	4:D:194:ALA:HB1	1.78	0.65
3:C:309:THR:HG21	3:C:367:PRO:O	1.97	0.64
3:C:78:ILE:CD1	5:E:57:GLN:HE21	2.11	0.64
3:C:100:ARG:HD3	16:C:1001:HOH:O	1.95	0.64
2:B:111:CYS:HB3	2:B:119:LEU:HD13	1.80	0.63
2:B:247:GLN:NE2	2:B:430:LEU:H	1.95	0.63
1:A:19:LEU:HB3	1:A:21:ASN:HB3	1.79	0.63
1:A:351:GLU:H	11:K:12:GLN:NE2	1.95	0.63
4:D:160:MET:HG2	4:D:161:ALA:H	1.64	0.63
3:C:78:ILE:HD13	5:E:57:GLN:NE2	2.14	0.62
1:A:276:ILE:HD13	1:A:353:GLU:HG3	1.80	0.62
5:E:51:ALA:O	5:E:55:VAL:HG23	1.99	0.62
3:C:186:PRO:HG2	12:C:381:HEC:HBB2	1.81	0.62
7:G:56:TYR:O	7:G:60:THR:HG22	2.00	0.62
1:A:308:GLN:HE21	1:A:323:HIS:CD2	2.14	0.62
2:B:78:LYS:HD2	2:B:129:ALA:HB1	1.81	0.62
3:C:94:LEU:HD21	3:C:123:VAL:HG11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:164:ILE:HG22	4:D:179:MET:HG2	1.82	0.61
3:C:26:ASN:HD22	3:C:207:ASN:HB2	1.64	0.61
5:E:50:ALA:O	5:E:54:VAL:HG23	1.99	0.61
1:A:417:ASP:O	5:E:33:LYS:HE3	2.00	0.61
1:A:233:PRO:HB2	5:E:22:THR:O	2.01	0.61
1:A:237:THR:CG2	5:E:14:ARG:NH2	2.63	0.61
3:C:3:ASN:HD22	3:C:6:LYS:HE2	1.64	0.61
9:I:29:LEU:O	9:I:32:ALA:HB3	2.01	0.61
3:C:137:GLN:HB2	3:C:254:ASP:O	2.00	0.60
2:B:99:THR:OG1	9:I:14:VAL:HG13	2.01	0.60
3:C:45:ILE:HA	12:C:381:HEC:HAB	1.83	0.60
2:B:76:THR:HG23	2:B:136:GLU:OE1	2.02	0.60
2:B:157:ALA:HA	9:I:11:PHE:CE1	2.36	0.59
2:B:232:LEU:HB2	2:B:234:GLY:HA3	1.83	0.59
3:C:267:HIS:HD2	3:C:269:LYS:HB3	1.68	0.59
1:A:149:VAL:HG21	1:A:252:HIS:HB3	1.84	0.59
1:A:281:ASP:HB2	9:I:20:ARG:HE	1.69	0.58
3:C:85:ASN:HD22	3:C:243:VAL:HG12	1.69	0.58
5:E:91:TRP:HZ3	5:E:136:ILE:HD11	1.68	0.58
1:A:281:ASP:OD1	9:I:47:ARG:HA	2.03	0.58
3:C:27:ILE:CD1	13:C:383:UQ2:H3M1	2.33	0.58
2:B:317:SER:OG	2:B:318:ASP:HB2	2.04	0.58
8:H:38:GLU:HA	8:H:41:ASP:HB2	1.85	0.58
2:B:200:THR:HG21	2:B:229:GLY:H	1.68	0.58
1:A:378:ASP:O	1:A:382:SER:HB2	2.04	0.58
3:C:206:ASN:ND2	3:C:207:ASN:H	2.02	0.58
1:A:60:GLU:OE2	2:B:287:ARG:NH2	2.27	0.57
12:C:382:HEC:HMC1	12:C:382:HEC:HBC2	1.87	0.57
2:B:353:SER:HB2	2:B:356:ASP:HB2	1.85	0.57
16:B:477:HOH:O	9:I:4:VAL:HB	2.04	0.57
1:A:46:ARG:HG3	1:A:163:LEU:HD13	1.86	0.57
1:A:432:PRO:HB2	1:A:437:ILE:HG13	1.85	0.57
3:C:78:ILE:HD11	5:E:57:GLN:HE21	1.70	0.56
6:F:78:GLU:HG3	16:F:1938:HOH:O	2.06	0.56
3:C:106:SER:HA	3:C:313:ARG:HH21	1.71	0.56
4:D:90:TYR:CB	4:D:92:PRO:HD2	2.35	0.56
3:C:228:ASP:OD2	13:C:383:UQ2:H5M3	2.06	0.56
5:E:70:ALA:C	5:E:72:SER:H	2.09	0.56
3:C:78:ILE:CD1	5:E:57:GLN:NE2	2.69	0.56
4:D:160:MET:HG2	4:D:161:ALA:N	2.21	0.56
9:I:11:PHE:HZ	9:I:27:ARG:HE	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:382:HEC:HBA1	12:C:382:HEC:HHA	1.88	0.55
1:A:146:ARG:NH1	1:A:308:GLN:HE22	2.04	0.55
2:B:245:ARG:NH2	2:B:433:THR:O	2.38	0.55
1:A:248:LEU:O	1:A:427:PRO:HG3	2.06	0.55
3:C:8:HIS:HD2	3:C:11:MET:H	1.54	0.55
13:C:383:UQ2:H5M1	13:C:383:UQ2:C8	2.36	0.55
3:C:105:GLY:HA2	3:C:107:TYR:CE1	2.42	0.54
3:C:308:HIS:O	3:C:309:THR:HG22	2.07	0.54
1:A:220:SER:HA	1:A:223:TYR:HB3	1.89	0.54
12:C:382:HEC:HMB1	12:C:382:HEC:HBB2	1.89	0.54
1:A:37:VAL:HG13	1:A:199:ALA:HB2	1.90	0.53
1:A:48:GLU:HG3	1:A:53:ASN:HD22	1.73	0.53
1:A:52:ASN:HA	1:A:177:LEU:HD21	1.91	0.53
2:B:39:GLU:OE2	2:B:41:TYR:HA	2.08	0.52
2:B:385:GLN:HE22	2:B:393:THR:N	2.08	0.52
3:C:27:ILE:HD11	13:C:383:UQ2:H3M1	1.91	0.52
5:E:65:SER:O	5:E:66:ALA:C	2.48	0.52
7:G:65:GLU:O	7:G:69:SER:HB2	2.09	0.52
5:E:70:ALA:O	5:E:72:SER:N	2.42	0.52
4:D:90:TYR:HB3	4:D:92:PRO:HD2	1.91	0.52
2:B:287:ARG:HA	9:I:34:VAL:HG13	1.91	0.52
3:C:35:SER:HB3	13:C:383:UQ2:CM5	2.37	0.51
5:E:73:LYS:O	5:E:74:ILE:HB	2.10	0.51
1:A:145:MET:O	1:A:149:VAL:HG23	2.10	0.51
4:D:165:TYR:HB2	4:D:179:MET:HG3	1.91	0.51
5:E:73:LYS:O	5:E:91:TRP:NE1	2.44	0.51
2:B:99:THR:HG23	9:I:14:VAL:HG22	1.92	0.51
2:B:68:LEU:HD23	2:B:186:VAL:HG22	1.92	0.51
3:C:237:LEU:HD13	4:D:212:MET:HG2	1.91	0.51
5:E:99:ARG:NH2	5:E:105:GLU:OE2	2.39	0.51
5:E:73:LYS:N	5:E:91:TRP:HE1	2.09	0.51
1:A:313:CYS:HB3	16:A:472:HOH:O	2.11	0.50
3:C:75:TYR:HB3	3:C:78:ILE:HD11	1.92	0.50
5:E:73:LYS:H	5:E:91:TRP:HE1	1.59	0.50
1:A:25:VAL:HG22	1:A:208:LEU:HD13	1.92	0.50
7:G:3:GLN:O	7:G:4:PHE:HB2	2.11	0.50
1:A:86:LEU:HD23	2:B:285:VAL:HG13	1.94	0.50
1:A:369:LEU:HD12	1:A:392:LEU:HD21	1.94	0.50
2:B:19:PRO:HB2	2:B:20:HIS:O	2.11	0.50
10:J:50:LYS:O	10:J:52:TRP:N	2.44	0.50
1:A:280:TYR:HA	1:A:284:TYR:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:349:THR:HA	3:C:352:GLN:HE21	1.76	0.50
6:F:82:LYS:O	6:F:84:GLU:O	2.30	0.50
2:B:129:ALA:N	2:B:130:PRO:HD2	2.25	0.50
3:C:51:LEU:HD13	3:C:79:ILE:HG22	1.94	0.50
1:A:237:THR:HG1	5:E:14:ARG:NH2	2.04	0.49
2:B:283:PRO:HD3	9:I:30:VAL:HB	1.93	0.49
3:C:150:LEU:HB2	3:C:161:VAL:HG13	1.93	0.49
4:D:19:SER:H	4:D:202:LYS:HD3	1.76	0.49
2:B:71:LEU:HD23	9:I:15:LEU:HG	1.94	0.49
3:C:5:ARG:NH2	3:C:20:ASP:OD1	2.46	0.49
3:C:124:MET:HG2	3:C:274:PHE:HE1	1.77	0.49
1:A:173:ASN:HA	1:A:176:LYS:HD3	1.95	0.49
3:C:15:ASN:HA	3:C:19:ILE:HG12	1.94	0.49
4:D:163:PRO:HG2	12:D:242:HEC:HBB2	1.95	0.49
1:A:252:HIS:CD2	1:A:323:HIS:HE1	2.31	0.48
2:B:265:GLY:HA2	16:B:491:HOH:O	2.13	0.48
3:C:359:PHE:O	3:C:363:LEU:HB2	2.13	0.48
3:C:361:LEU:HA	3:C:365:LEU:HB2	1.94	0.48
5:E:65:SER:C	5:E:67:ASP:N	2.65	0.48
3:C:50:PHE:CE2	5:E:62:MET:HE2	2.48	0.48
6:F:28:LYS:HB3	6:F:74:ILE:CG1	2.44	0.48
1:A:443:TRP:HB3	1:A:445:ARG:HG2	1.95	0.48
6:F:35:ASP:OD1	6:F:61:ARG:HD2	2.13	0.48
9:I:5:ALA:O	9:I:8:SER:N	2.45	0.48
3:C:146:ILE:HG13	14:C:384:OST:C12	2.44	0.48
2:B:37:SER:HA	2:B:208:GLY:O	2.13	0.48
5:E:73:LYS:O	5:E:91:TRP:CD1	2.67	0.48
6:F:42:ASP:OD2	6:F:101:ARG:NH1	2.46	0.48
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.95	0.48
7:G:72:LYS:HD3	7:G:73:ASN:H	1.79	0.48
1:A:280:TYR:CG	1:A:281:ASP:N	2.82	0.47
1:A:281:ASP:OD2	9:I:47:ARG:HG2	2.14	0.47
1:A:373:THR:HB	1:A:374:PRO:HD3	1.96	0.47
5:E:99:ARG:HH12	5:E:155:GLY:HA2	1.79	0.47
2:B:241:GLY:HA2	2:B:423:SER:OG	2.14	0.47
2:B:343:GLN:O	2:B:346:THR:HG22	2.15	0.47
5:E:73:LYS:O	5:E:74:ILE:CB	2.62	0.47
1:A:158:PHE:O	1:A:164:ALA:HB2	2.15	0.47
3:C:107:TYR:OH	3:C:308:HIS:ND1	2.35	0.47
1:A:2:ALA:O	2:B:113:ARG:HD3	2.14	0.47
1:A:149:VAL:HG21	1:A:252:HIS:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:CYS:CB	16:A:472:HOH:O	2.62	0.47
3:C:44:GLN:HG3	12:C:381:HEC:HBC2	1.96	0.47
8:H:73:LEU:O	8:H:75:ASN:N	2.33	0.47
2:B:397:THR:HA	2:B:400:GLN:HB3	1.97	0.47
3:C:186:PRO:HA	3:C:189:ILE:HB	1.97	0.47
4:D:116:ILE:HG22	4:D:190:LEU:HD22	1.97	0.47
1:A:156:THR:O	1:A:159:GLN:HG2	2.15	0.47
2:B:253:VAL:HG23	2:B:330:ALA:HA	1.96	0.47
1:A:378:ASP:OD2	1:A:389:ARG:NH1	2.47	0.46
5:E:65:SER:O	5:E:67:ASP:N	2.48	0.46
1:A:29:GLN:HB2	1:A:203:LEU:O	2.16	0.46
3:C:216:ASP:OD2	4:D:233:ARG:NH2	2.47	0.46
2:B:344:VAL:HG11	2:B:417:PHE:CD2	2.50	0.46
9:I:42:VAL:HA	9:I:46:LYS:HZ2	1.80	0.46
4:D:21:LEU:HD21	4:D:191:ARG:HG2	1.98	0.46
2:B:95:LYS:HD2	2:B:110:GLU:OE2	2.15	0.46
8:H:18:THR:HA	8:H:21:ARG:HB2	1.97	0.46
7:G:73:ASN:CB	7:G:74:PRO:HD3	2.40	0.46
5:E:23:LYS:HG3	5:E:24:SER:H	1.81	0.46
4:D:180:SER:HB2	8:H:77:LEU:HD21	1.98	0.45
3:C:268:ILE:HG22	14:C:384:OST:H9	1.97	0.45
5:E:171:ILE:HD13	5:E:176:ALA:HB3	1.98	0.45
3:C:378:LYS:HE2	6:F:17:ARG:HD3	1.99	0.45
1:A:376:CYS:HA	1:A:379:ILE:HD12	1.99	0.45
1:A:30:SER:HA	2:B:18:PRO:HG3	1.98	0.45
2:B:325:TYR:HD2	9:I:28:PRO:HG2	1.82	0.45
3:C:104:TYR:CD2	3:C:208:PRO:HA	2.52	0.45
5:E:53:ASN:O	5:E:57:GLN:HG3	2.16	0.45
3:C:77:TRP:CZ3	3:C:78:ILE:HG23	2.51	0.45
2:B:353:SER:HB2	2:B:356:ASP:CB	2.46	0.44
2:B:394:PRO:HD2	2:B:397:THR:HG23	1.99	0.44
3:C:294:LEU:HD11	14:C:384:OST:H18	1.99	0.44
8:H:36:ARG:HA	8:H:39:LEU:HB2	1.98	0.44
6:F:68:LEU:HD23	6:F:71:ARG:NH1	2.28	0.44
3:C:152:ALA:HB2	3:C:287:LYS:HE2	1.99	0.44
6:F:43:VAL:O	6:F:47:ILE:HG12	2.18	0.44
1:A:310:PHE:CD1	1:A:312:ILE:HD12	2.53	0.44
2:B:129:ALA:N	2:B:130:PRO:CD	2.80	0.44
4:D:181:GLN:HE21	8:H:77:LEU:HD13	1.82	0.44
8:H:15:ASP:HA	8:H:16:PRO:HD3	1.88	0.44
8:H:40:CYS:HA	8:H:43:ARG:HE	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:ASN:HD22	2:B:238:LYS:HG3	1.83	0.44
2:B:124:LEU:HD11	2:B:219:VAL:HG13	2.00	0.44
1:A:341:GLN:HE22	1:A:344:ARG:HE	1.66	0.44
9:I:11:PHE:HD2	9:I:11:PHE:HA	1.72	0.44
1:A:45:SER:HB3	1:A:92:ARG:HA	1.99	0.43
1:A:83:GLY:HA2	2:B:363:LYS:HG2	2.00	0.43
1:A:359:ASN:ND2	1:A:362:ARG:HH11	2.16	0.43
4:D:164:ILE:HD11	12:D:242:HEC:HBB1	2.00	0.43
1:A:252:HIS:CD2	1:A:323:HIS:CE1	3.06	0.43
5:E:64:ALA:HB1	5:E:69:LEU:HG	2.00	0.43
5:E:96:LEU:HD21	5:E:195:VAL:HG21	2.01	0.43
3:C:206:ASN:HD22	3:C:207:ASN:H	1.63	0.43
3:C:237:LEU:HD22	4:D:216:LEU:HD11	2.00	0.43
13:C:383:UQ2:H2M3	13:C:383:UQ2:H3M2	2.00	0.43
4:D:201:ARG:HH21	4:D:202:LYS:HE3	1.83	0.43
1:A:45:SER:HA	1:A:48:GLU:CG	2.47	0.43
2:B:385:GLN:HE22	2:B:393:THR:H	1.64	0.43
10:J:21:ALA:O	10:J:25:VAL:HG23	2.18	0.43
3:C:74:ASN:HD21	5:E:64:ALA:HB3	1.82	0.43
2:B:264:ILE:HG12	9:I:2:LEU:HD23	2.00	0.43
5:E:14:ARG:HD3	5:E:18:VAL:O	2.19	0.43
3:C:218:ILE:HG21	4:D:230:LEU:HD11	2.00	0.43
3:C:318:ARG:HB2	3:C:373:GLU:OE1	2.19	0.43
4:D:47:ALA:HB2	4:D:90:TYR:CD2	2.53	0.43
4:D:181:GLN:HG2	8:H:77:LEU:HD22	1.99	0.43
6:F:37:ILE:HD12	6:F:43:VAL:HG21	2.00	0.43
4:D:201:ARG:NH2	4:D:202:LYS:HE3	2.34	0.43
7:G:26:PHE:HB3	7:G:29:TYR:HB2	2.01	0.43
1:A:49:SER:HB2	1:A:51:LYS:O	2.19	0.42
3:C:87:ALA:HA	12:C:381:HEC:HBC3	2.01	0.42
5:E:52:LYS:O	5:E:53:ASN:C	2.56	0.42
5:E:145:VAL:HA	5:E:146:PRO:HD3	1.91	0.42
1:A:102:LEU:HD23	1:A:104:LYS:HE2	2.01	0.42
1:A:196:VAL:HG21	1:A:383:LEU:HB3	2.00	0.42
2:B:395:PRO:O	2:B:399:LEU:HG	2.19	0.42
4:D:110:PRO:HA	4:D:111:PRO:HD2	1.95	0.42
1:A:255:ILE:HD12	1:A:422:VAL:HG22	2.00	0.42
3:C:131:TYR:HA	12:C:381:HEC:HAD2	2.01	0.42
13:C:383:UQ2:H5M1	13:C:383:UQ2:C9	2.50	0.42
3:C:326:TRP:CD2	7:G:48:VAL:HG13	2.54	0.42
3:C:126:THR:OG1	3:C:185:LEU:HD23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:217:LYS:HG3	7:G:7:LEU:HD13	2.02	0.42
3:C:222:PRO:HB2	4:D:226:LYS:HG2	2.02	0.42
5:E:72:SER:HB3	5:E:92:ARG:NE	2.22	0.42
2:B:40:ASN:O	2:B:40:ASN:ND2	2.53	0.42
2:B:208:GLY:HA3	2:B:216:LEU:HD11	2.02	0.42
3:C:100:ARG:HH12	12:C:382:HEC:HBD2	1.85	0.42
3:C:100:ARG:NH1	12:C:382:HEC:HBD2	2.34	0.42
5:E:16:PRO:C	5:E:18:VAL:H	2.23	0.42
1:A:36:THR:O	1:A:199:ALA:HA	2.20	0.42
6:F:82:LYS:C	6:F:84:GLU:O	2.58	0.42
4:D:23:HIS:CE1	10:J:50:LYS:HG3	2.55	0.41
6:F:65:ALA:HA	6:F:68:LEU:HD12	2.02	0.41
4:D:30:PHE:CE2	4:D:64:LEU:HD13	2.55	0.41
6:F:28:LYS:HB3	6:F:74:ILE:HG13	2.01	0.41
5:E:171:ILE:CD1	5:E:176:ALA:HB3	2.50	0.41
5:E:45:VAL:HG13	10:J:28:ALA:HA	2.02	0.41
6:F:27:ASN:HA	6:F:81:THR:HG23	2.03	0.41
3:C:146:ILE:HD11	14:C:384:OST:H8	2.03	0.41
3:C:246:ALA:HB1	3:C:249:LEU:HB2	2.03	0.41
3:C:300:ILE:HD11	3:C:363:LEU:HD13	2.03	0.41
3:C:332:LEU:O	3:C:336:THR:HG23	2.21	0.41
1:A:198:ALA:HB2	1:A:380:GLY:H	1.85	0.41
3:C:8:HIS:CD2	3:C:11:MET:H	2.37	0.41
5:E:70:ALA:C	5:E:72:SER:N	2.74	0.41
2:B:25:GLU:O	2:B:36:ALA:HA	2.21	0.41
4:D:225:HIS:CE1	7:G:20:PRO:HB2	2.55	0.41
4:D:227:TRP:O	4:D:231:LYS:HG2	2.21	0.41
9:I:15:LEU:HD22	9:I:15:LEU:HA	1.88	0.41
1:A:8:LEU:HD22	1:A:392:LEU:HB3	2.03	0.40
1:A:244:ARG:NH2	16:A:450:HOH:O	2.34	0.40
3:C:117:VAL:N	12:C:382:HEC:HBC3	2.36	0.40
8:H:62:LEU:HD23	8:H:65:ARG:HH12	1.86	0.40
3:C:223:TYR:HB3	4:D:227:TRP:CZ2	2.56	0.40
5:E:17:GLU:HB3	5:E:28:SER:CB	2.51	0.40
4:D:41:HIS:ND1	4:D:113:LEU:HD13	2.36	0.40
5:E:33:LYS:O	5:E:34:GLY:C	2.60	0.40
1:A:270:LEU:HD22	1:A:320:LEU:HD21	2.04	0.40
1:A:418:GLN:HE21	1:A:418:GLN:HA	1.86	0.40
4:D:23:HIS:HA	4:D:26:ILE:HD12	2.02	0.40
11:K:33:VAL:HG22	11:K:41:ILE:HD13	2.04	0.40
3:C:153:ILE:HA	3:C:154:PRO:HD3	1.97	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	444/446 (100%)	393 (88%)	34 (8%)	17 (4%)	3 18
2	B	421/439 (96%)	377 (90%)	31 (7%)	13 (3%)	4 23
3	C	376/379 (99%)	321 (85%)	41 (11%)	14 (4%)	3 19
4	D	239/241 (99%)	187 (78%)	33 (14%)	19 (8%)	1 4
5	E	194/196 (99%)	174 (90%)	12 (6%)	8 (4%)	3 16
6	F	103/110 (94%)	91 (88%)	10 (10%)	2 (2%)	8 36
7	G	73/81 (90%)	66 (90%)	4 (6%)	3 (4%)	3 16
8	H	68/78 (87%)	56 (82%)	7 (10%)	5 (7%)	1 5
9	I	55/78 (70%)	24 (44%)	20 (36%)	11 (20%)	0 0
10	J	57/62 (92%)	45 (79%)	6 (10%)	6 (10%)	0 2
11	K	52/56 (93%)	45 (86%)	5 (10%)	2 (4%)	3 18
All	All	2082/2166 (96%)	1779 (85%)	203 (10%)	100 (5%)	2 13

All (100) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	46	ARG
1	A	121	SER
1	A	223	TYR
1	A	224	ASP
1	A	226	ASP
1	A	239	SER
1	A	288	ALA
1	A	357	GLY
2	B	21	PRO

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Mol	Chain	Res	Type
2	B	232	LEU
2	B	250	ASP
2	B	305	GLN
2	B	437	ASP
3	C	109	PHE
3	C	206	ASN
3	C	263	ASN
3	C	347	TYR
4	D	89	ASP
4	D	92	PRO
4	D	121	HIS
4	D	154	PRO
4	D	161	ALA
4	D	166	ASN
4	D	175	THR
4	D	182	VAL
4	D	198	HIS
5	E	64	ALA
5	E	65	SER
5	E	69	LEU
5	E	71	MET
5	E	73	LYS
5	E	74	ILE
7	G	73	ASN
8	H	12	GLU
8	H	26	GLN
8	H	73	LEU
8	H	74	PHE
9	I	5	ALA
9	I	8	SER
9	I	27	ARG
9	I	34	VAL
9	I	40	SER
9	I	43	LEU
9	I	50	LEU
10	J	18	SER
10	J	37	GLN
10	J	51	LEU
10	J	54	HIS
11	K	4	ARG
11	K	49	ASN
1	A	45	SER

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Mol	Chain	Res	Type
2	B	54	GLY
2	B	79	GLY
2	B	249	GLY
2	B	436	ILE
3	C	12	LYS
3	C	142	GLY
3	C	257	THR
3	C	346	PRO
4	D	24	THR
4	D	80	MET
4	D	139	THR
4	D	143	LEU
5	E	67	ASP
6	F	87	LYS
7	G	4	PHE
8	H	42	GLU
9	I	41	PRO
9	I	45	LEU
10	J	44	GLU
1	A	304	CYS
1	A	379	ILE
1	A	380	GLY
2	B	52	LYS
3	C	156	ILE
3	C	177	ARG
4	D	71	GLN
4	D	111	PRO
7	G	71	ARG
1	A	218	GLY
1	A	238	GLY
2	B	236	LYS
2	B	319	SER
3	C	254	ASP
3	C	264	THR
4	D	49	ARG
5	E	66	ALA
1	A	42	ASP
3	C	21	LEU
3	C	266	PRO
6	F	84	GLU
9	I	53	GLU
4	D	162	PRO

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Mol	Chain	Res	Type
4	D	170	GLU
10	J	36	ASP
1	A	233	PRO
4	D	93	LYS
2	B	20	HIS
9	I	9	GLY

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	Percentiles
1	A	370/370 (100%)	304 (82%)	66 (18%)	2 9
2	B	332/343 (97%)	292 (88%)	40 (12%)	5 22
3	C	326/327 (100%)	270 (83%)	56 (17%)	2 10
4	D	206/206 (100%)	156 (76%)	50 (24%)	0 3
5	E	168/168 (100%)	157 (94%)	11 (6%)	17 50
6	F	96/98 (98%)	77 (80%)	19 (20%)	1 7
7	G	66/71 (93%)	54 (82%)	12 (18%)	1 9
8	H	67/74 (90%)	43 (64%)	24 (36%)	0 1
9	I	44/60 (73%)	26 (59%)	18 (41%)	0 0
10	J	50/52 (96%)	38 (76%)	12 (24%)	0 3
11	K	44/46 (96%)	33 (75%)	11 (25%)	0 3
All	All	1769/1815 (98%)	1450 (82%)	319 (18%)	1 9

All (319) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	9	GLN
1	A	13	GLU
1	A	17	SER
1	A	19	LEU

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Mol	Chain	Res	Type
1	A	23	LEU
1	A	24	ARG
1	A	29	GLN
1	A	32	GLN
1	A	34	THR
1	A	37	VAL
1	A	48	GLU
1	A	52	ASN
1	A	58	PHE
1	A	68	LYS
1	A	90	SER
1	A	104	LYS
1	A	108	LYS
1	A	117	VAL
1	A	127	ILE
1	A	128	GLU
1	A	131	ARG
1	A	136	GLN
1	A	140	GLU
1	A	143	THR
1	A	146	ARG
1	A	163	LEU
1	A	176	LYS
1	A	179	ARG
1	A	183	THR
1	A	184	GLU
1	A	186	LEU
1	A	187	SER
1	A	188	ARG
1	A	191	LYS
1	A	194	ARG
1	A	203	LEU
1	A	204	GLU
1	A	207	GLN
1	A	208	LEU
1	A	209	LEU
1	A	214	LYS
1	A	217	SER
1	A	222	THR
1	A	225	GLU
1	A	230	THR
1	A	231	LEU

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Mol	Chain	Res	Type
1	A	245	GLU
1	A	255	ILE
1	A	274	ASN
1	A	296	SER
1	A	300	THR
1	A	304	CYS
1	A	313	CYS
1	A	367	SER
1	A	381	ARG
1	A	382	SER
1	A	383	LEU
1	A	388	ARG
1	A	389	ARG
1	A	392	LEU
1	A	397	SER
1	A	403	ASP
1	A	418	GLN
1	A	438	ARG
1	A	439	SER
2	B	17	VAL
2	B	20	HIS
2	B	33	LEU
2	B	38	LEU
2	B	40	ASN
2	B	46	ARG
2	B	69	LEU
2	B	76	THR
2	B	97	SER
2	B	98	VAL
2	B	104	ASN
2	B	109	VAL
2	B	110	GLU
2	B	119	LEU
2	B	123	LEU
2	B	163	LEU
2	B	175	SER
2	B	176	LEU
2	B	186	VAL
2	B	189	VAL
2	B	197	ASN
2	B	227	ARG
2	B	230	LEU

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Mol	Chain	Res	Type
2	B	232	LEU
2	B	248	ASN
2	B	257	LEU
2	B	258	VAL
2	B	264	ILE
2	B	273	SER
2	B	294	SER
2	B	309	VAL
2	B	329	GLN
2	B	346	THR
2	B	353	SER
2	B	358	GLN
2	B	379	LEU
2	B	397	THR
2	B	422	LYS
2	B	435	PHE
2	B	437	ASP
3	C	2	THR
3	C	4	ILE
3	C	12	LYS
3	C	39	ILE
3	C	41	LEU
3	C	51	LEU
3	C	56	THR
3	C	59	THR
3	C	60	THR
3	C	64	SER
3	C	74	ASN
3	C	78	ILE
3	C	80	ARG
3	C	88	SER
3	C	90	PHE
3	C	94	LEU
3	C	96	MET
3	C	100	ARG
3	C	102	LEU
3	C	134	PRO
3	C	145	VAL
3	C	160	LEU
3	C	161	VAL
3	C	164	ILE
3	C	171	ASP

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Mol	Chain	Res	Type
3	C	174	THR
3	C	175	LEU
3	C	176	THR
3	C	183	PHE
3	C	190	MET
3	C	194	MET
3	C	205	SER
3	C	206	ASN
3	C	212	SER
3	C	227	LYS
3	C	243	VAL
3	C	254	ASP
3	C	257	THR
3	C	262	LEU
3	C	269	LYS
3	C	276	PHE
3	C	284	ILE
3	C	300	ILE
3	C	303	LEU
3	C	306	LEU
3	C	307	LEU
3	C	309	THR
3	C	320	LEU
3	C	321	SER
3	C	324	LEU
3	C	328	LEU
3	C	334	THR
3	C	336	THR
3	C	350	ILE
3	C	378	LYS
3	C	379	TRP
4	D	2	ASP
4	D	3	LEU
4	D	5	LEU
4	D	9	SER
4	D	13	SER
4	D	15	ARG
4	D	17	LEU
4	D	24	THR
4	D	34	LYS
4	D	39	SER
4	D	42	SER

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Mol	Chain	Res	Type
4	D	43	MET
4	D	55	CYS
4	D	62	LYS
4	D	66	GLU
4	D	68	VAL
4	D	72	ASP
4	D	75	ASN
4	D	79	GLU
4	D	80	MET
4	D	82	MET
4	D	83	ARG
4	D	116	ILE
4	D	118	ARG
4	D	120	ARG
4	D	124	GLU
4	D	130	LEU
4	D	132	THR
4	D	139	THR
4	D	141	VAL
4	D	143	LEU
4	D	145	GLU
4	D	158	ILE
4	D	165	TYR
4	D	166	ASN
4	D	169	LEU
4	D	172	ASP
4	D	173	ASP
4	D	179	MET
4	D	181	GLN
4	D	186	VAL
4	D	190	LEU
4	D	191	ARG
4	D	201	ARG
4	D	211	MET
4	D	214	LEU
4	D	223	LYS
4	D	226	LYS
4	D	234	LYS
4	D	241	LYS
5	E	20	ASP
5	E	22	THR
5	E	23	LYS

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Mol	Chain	Res	Type
5	E	52	LYS
5	E	60	SER
5	E	65	SER
5	E	67	ASP
5	E	113	GLU
5	E	135	LEU
5	E	188	THR
5	E	189	SER
6	F	7	SER
6	F	11	ARG
6	F	12	TRP
6	F	22	ASN
6	F	33	ARG
6	F	37	ILE
6	F	53	ASN
6	F	64	ARG
6	F	71	ARG
6	F	73	GLN
6	F	74	ILE
6	F	78	GLU
6	F	81	THR
6	F	84	GLU
6	F	90	LEU
6	F	94	LEU
6	F	99	ARG
6	F	105	GLU
6	F	110	LYS
7	G	8	THR
7	G	31	SER
7	G	34	ILE
7	G	36	ASN
7	G	37	VAL
7	G	42	ARG
7	G	44	CYS
7	G	45	ILE
7	G	53	VAL
7	G	60	THR
7	G	67	GLU
7	G	72	LYS
8	H	10	GLU
8	H	12	GLU
8	H	13	LEU

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Mol	Chain	Res	Type
8	H	14	VAL
8	H	18	THR
8	H	20	VAL
8	H	29	LYS
8	H	34	ARG
8	H	36	ARG
8	H	39	LEU
8	H	42	GLU
8	H	47	ARG
8	H	49	GLN
8	H	52	GLU
8	H	53	ASP
8	H	54	CYS
8	H	55	THR
8	H	56	GLU
8	H	58	LEU
8	H	60	ASP
8	H	65	ARG
8	H	68	CYS
8	H	72	LYS
8	H	77	LEU
9	I	1	MET
9	I	7	ARG
9	I	8	SER
9	I	15	LEU
9	I	16	SER
9	I	18	THR
9	I	26	LEU
9	I	27	ARG
9	I	30	VAL
9	I	31	GLN
9	I	37	THR
9	I	39	GLU
9	I	44	ASP
9	I	45	LEU
9	I	47	ARG
9	I	50	LEU
9	I	55	LEU
9	I	56	ARG
10	J	4	THR
10	J	5	LEU
10	J	9	LEU

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Mol	Chain	Res	Type
10	J	12	LEU
10	J	18	SER
10	J	24	ILE
10	J	29	LEU
10	J	48	GLU
10	J	54	HIS
10	J	55	ILE
10	J	56	LYS
10	J	60	GLU
11	K	1	MET
11	K	2	LEU
11	K	6	LEU
11	K	13	LEU
11	K	23	LEU
11	K	24	TRP
11	K	38	TRP
11	K	40	LEU
11	K	44	TRP
11	K	52	PHE
11	K	54	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	53	ASN
1	A	141	ASN
1	A	173	ASN
1	A	189	HIS
1	A	252	HIS
1	A	274	ASN
1	A	323	HIS
1	A	341	GLN
1	A	359	ASN
1	A	418	GLN
2	B	40	ASN
2	B	153	GLN
2	B	170	ASN
2	B	174	ASN
2	B	247	GLN
2	B	276	GLN
2	B	277	HIS

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Mol	Chain	Res	Type
2	B	284	HIS
2	B	342	ASN
2	B	343	GLN
2	B	385	GLN
3	C	3	ASN
3	C	8	HIS
3	C	26	ASN
3	C	32	ASN
3	C	68	HIS
3	C	74	ASN
3	C	85	ASN
3	C	114	ASN
3	C	201	HIS
3	C	206	ASN
3	C	267	HIS
3	C	352	GLN
4	D	105	ASN
4	D	181	GLN
4	D	200	HIS
4	D	225	HIS
5	E	57	GLN
6	F	53	ASN
6	F	73	GLN
7	G	23	GLN
9	I	31	GLN
11	K	12	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
15	FES	E	197	5	0,4,4	-	-	-		
13	UQ2	C	383	-	23,23,23	2.87	8 (34%)	28,31,31	1.25	4 (14%)
14	OST	C	384	-	23,23,23	2.10	10 (43%)	29,29,29	1.43	6 (20%)
12	HEC	C	382	3	32,50,50	1.86	6 (18%)	24,82,82	1.68	7 (29%)
12	HEC	D	242	4	32,50,50	1.99	10 (31%)	24,82,82	1.68	5 (20%)
12	HEC	C	381	3	32,50,50	2.00	8 (25%)	24,82,82	1.44	4 (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
15	FES	E	197	5	-	-	0/1/1/1
13	UQ2	C	383	-	-	7/15/39/39	0/1/1/1
14	OST	C	384	-	-	5/18/18/18	0/2/2/2
12	HEC	C	382	3	-	9/10/54/54	-
12	HEC	D	242	4	-	3/10/54/54	-
12	HEC	C	381	3	-	3/10/54/54	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	383	UQ2	C6-C5	8.81	1.51	1.35
12	D	242	HEC	C2B-C3B	-6.40	1.34	1.40
12	C	381	HEC	C3C-C2C	-6.12	1.34	1.40
13	C	383	UQ2	C8-C9	4.89	1.44	1.33
12	C	382	HEC	CBA-CGA	-4.81	1.39	1.50
12	C	382	HEC	C2B-C3B	-4.63	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	382	HEC	CBD-CGD	-4.48	1.40	1.50
12	C	381	HEC	C2B-C3B	-4.28	1.36	1.40
14	C	384	OST	C6-C7	4.26	1.47	1.41
13	C	383	UQ2	C3-C2	4.26	1.53	1.36
13	C	383	UQ2	C7-C8	4.25	1.56	1.50
12	D	242	HEC	C3C-C2C	-4.25	1.36	1.40
14	C	384	OST	C11-C6	3.95	1.46	1.39
12	C	382	HEC	C3C-C2C	-3.83	1.36	1.40
12	C	381	HEC	CBD-CGD	-3.76	1.41	1.50
13	C	383	UQ2	C7-C6	3.39	1.57	1.51
13	C	383	UQ2	C13-C14	3.16	1.41	1.32
12	D	242	HEC	CBD-CGD	-2.97	1.43	1.50
14	C	384	OST	C15-C14	2.94	1.45	1.39
12	C	381	HEC	CAD-C3D	2.83	1.56	1.52
13	C	383	UQ2	C6-C1	2.81	1.54	1.46
12	C	381	HEC	CBA-CGA	-2.78	1.44	1.50
12	C	381	HEC	C4B-C3B	2.73	1.48	1.43
14	C	384	OST	O2-C3	-2.66	1.29	1.34
12	D	242	HEC	CAD-C3D	2.64	1.55	1.52
12	D	242	HEC	CAA-C2A	2.60	1.56	1.52
14	C	384	OST	C6-C2	2.58	1.52	1.49
13	C	383	UQ2	O2-C2	2.56	1.43	1.36
12	C	381	HEC	C2A-C1A	2.39	1.48	1.42
14	C	384	OST	C17-C18	2.33	1.44	1.38
12	D	242	HEC	C3A-C4A	2.32	1.47	1.42
14	C	384	OST	C16-C15	2.31	1.43	1.38
12	D	242	HEC	CBA-CGA	-2.27	1.45	1.50
12	D	242	HEC	C2A-C1A	2.23	1.47	1.42
14	C	384	OST	C17-C16	2.21	1.43	1.38
12	C	381	HEC	C1B-NB	2.19	1.40	1.36
14	C	384	OST	C18-C19	2.15	1.43	1.38
12	D	242	HEC	C3C-C4C	2.14	1.46	1.43
12	C	382	HEC	O2D-CGD	-2.14	1.23	1.30
14	C	384	OST	C10-C11	2.12	1.43	1.38
12	C	382	HEC	O2A-CGA	-2.06	1.23	1.30
12	D	242	HEC	CBC-CAC	2.01	1.57	1.49

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	D	242	HEC	CBA-CAA-C2A	4.39	120.01	112.60
12	C	382	HEC	CMC-C2C-C3C	3.42	129.84	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	382	HEC	CMC-C2C-C1C	-3.28	123.42	128.46
14	C	384	OST	C11-C6-C7	-2.78	115.81	119.25
12	D	242	HEC	O2A-CGA-O1A	-2.70	116.56	123.30
14	C	384	OST	C3-C2-C1	-2.69	112.47	117.41
13	C	383	UQ2	C7-C6-C1	2.68	121.71	118.48
13	C	383	UQ2	C6-C5-C4	2.63	121.26	119.18
12	D	242	HEC	C2B-C3B-C4B	2.59	109.14	106.35
12	C	382	HEC	O2A-CGA-CBA	2.57	122.30	114.03
12	C	382	HEC	CBA-CAA-C2A	2.57	116.94	112.60
12	C	382	HEC	CMB-C2B-C1B	-2.56	124.53	128.46
12	C	381	HEC	C2B-C3B-C4B	2.55	109.11	106.35
12	C	381	HEC	CBD-CAD-C3D	-2.54	108.28	112.62
13	C	383	UQ2	CM5-C5-C6	-2.54	120.26	124.40
14	C	384	OST	O1-C1-C2	2.52	115.71	112.01
12	C	381	HEC	C4C-C3C-C2C	2.42	108.96	106.35
12	D	242	HEC	O2D-CGD-CBD	2.39	121.71	114.03
12	C	382	HEC	CAD-C3D-C2D	-2.34	120.53	127.25
12	C	382	HEC	CMB-C2B-C3B	2.24	128.46	125.82
13	C	383	UQ2	C16-C14-C15	2.14	119.34	114.60
14	C	384	OST	C4-O2-C3	-2.12	111.91	115.61
12	D	242	HEC	O2A-CGA-CBA	2.12	120.85	114.03
12	C	381	HEC	O2A-CGA-CBA	2.09	120.74	114.03
14	C	384	OST	O1-C1-O3	-2.02	119.64	123.53
14	C	384	OST	C6-C2-C3	2.01	125.19	122.26

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	382	HEC	C1A-C2A-CAA-CBA
12	C	382	HEC	C3A-C2A-CAA-CBA
12	C	382	HEC	C2D-C3D-CAD-CBD
12	C	382	HEC	C4D-C3D-CAD-CBD
12	D	242	HEC	C1A-C2A-CAA-CBA
14	C	384	OST	C1-C2-C3-O2
13	C	383	UQ2	C9-C11-C12-C13
12	C	382	HEC	C3D-CAD-CBD-CGD
12	C	381	HEC	C3D-CAD-CBD-CGD
13	C	383	UQ2	C12-C11-C9-C10
13	C	383	UQ2	C1-C6-C7-C8
14	C	384	OST	O3-C1-C2-C6
13	C	383	UQ2	C12-C11-C9-C8

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Mol	Chain	Res	Type	Atoms
14	C	384	OST	O3-C1-C2-C3
14	C	384	OST	C12-C13-C14-C15
13	C	383	UQ2	C5-C6-C7-C8
13	C	383	UQ2	C1-C2-O2-CM2
12	C	381	HEC	CAD-CBD-CGD-O1D
12	D	242	HEC	CAD-CBD-CGD-O1D
12	D	242	HEC	CAD-CBD-CGD-O2D
12	C	382	HEC	CAD-CBD-CGD-O2D
12	C	382	HEC	CAA-CBA-CGA-O1A
12	C	381	HEC	CAD-CBD-CGD-O2D
12	C	382	HEC	CAA-CBA-CGA-O2A
12	C	382	HEC	CAD-CBD-CGD-O1D
14	C	384	OST	C12-C13-C14-C19
13	C	383	UQ2	C3-C2-O2-CM2

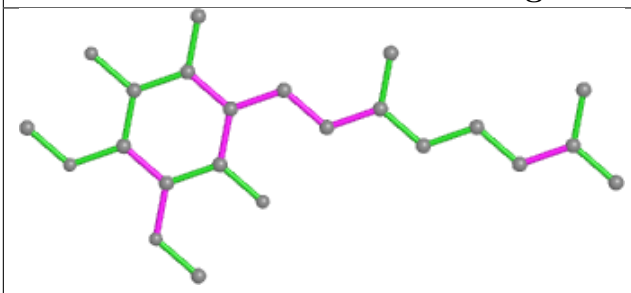
There are no ring outliers.

5 monomers are involved in 27 short contacts:

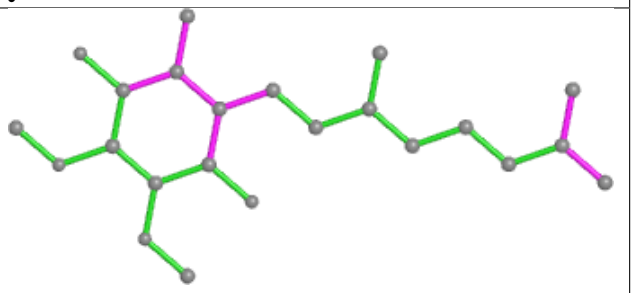
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	383	UQ2	8	0
14	C	384	OST	4	0
12	C	382	HEC	7	0
12	D	242	HEC	3	0
12	C	381	HEC	5	0

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.

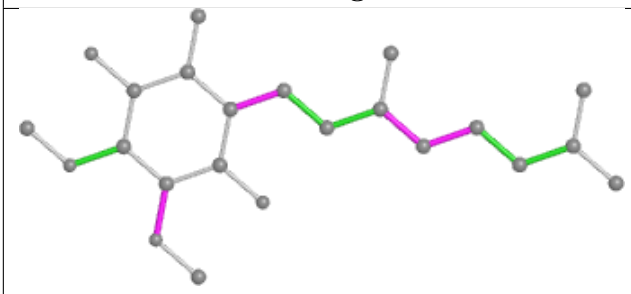
Ligand UQ2 C 383



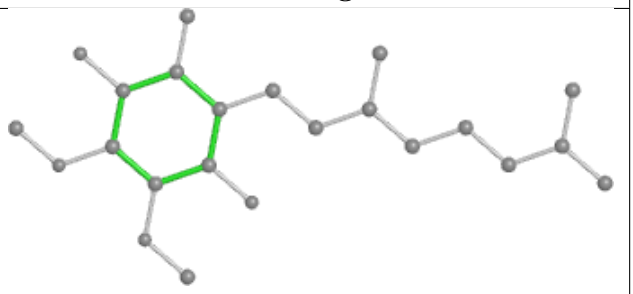
Bond lengths



Bond angles

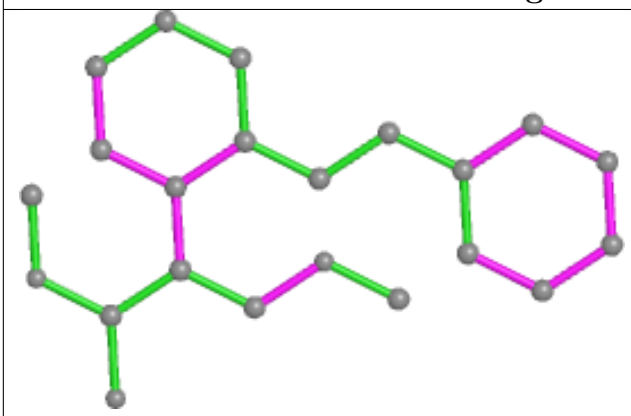


Torsions

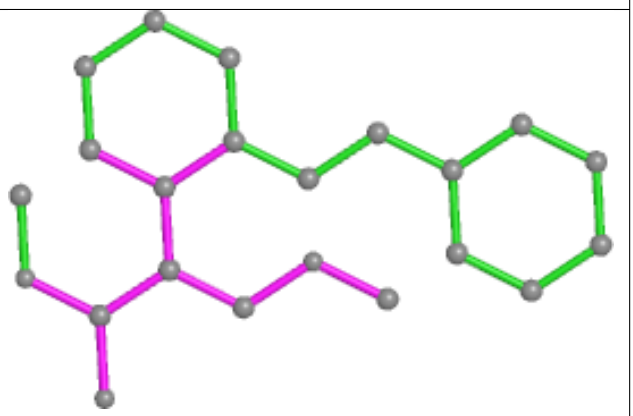


Rings

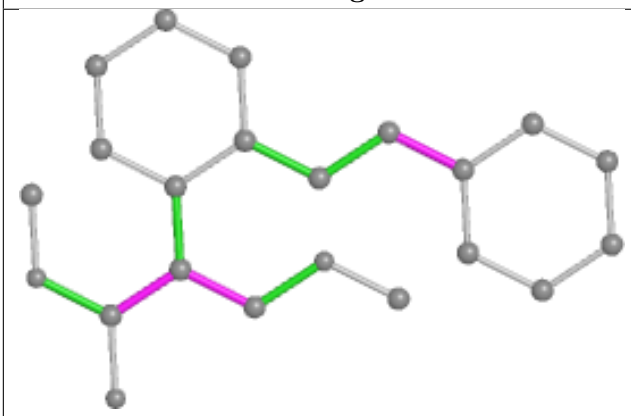
Ligand OST C 384



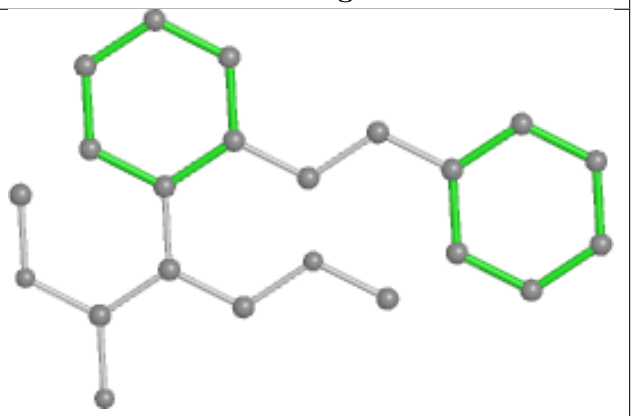
Bond lengths



Bond angles

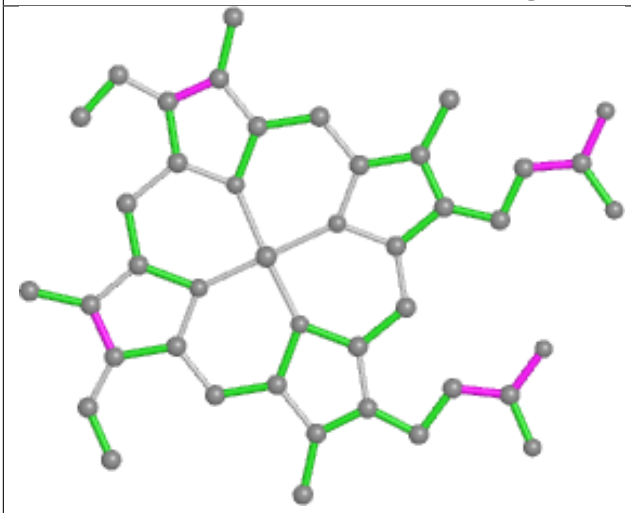


Torsions

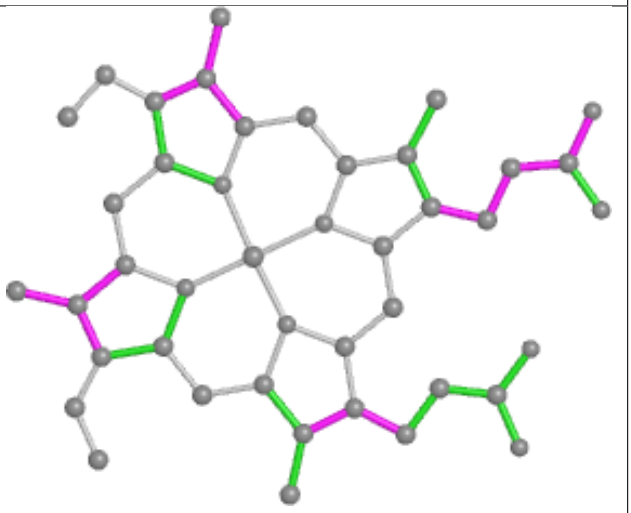


Rings

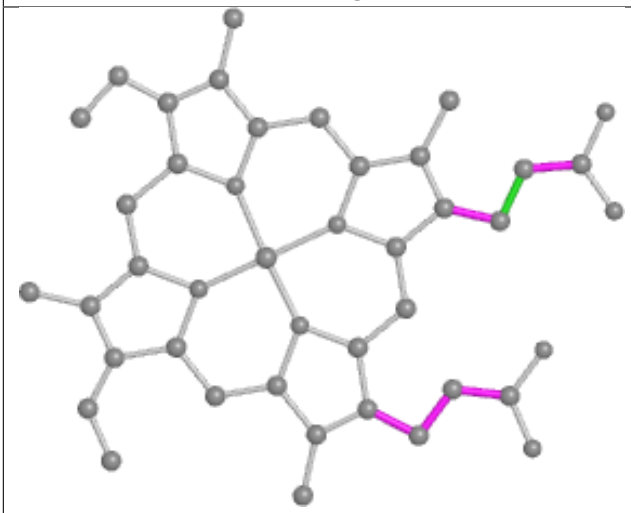
Ligand HEC C 382



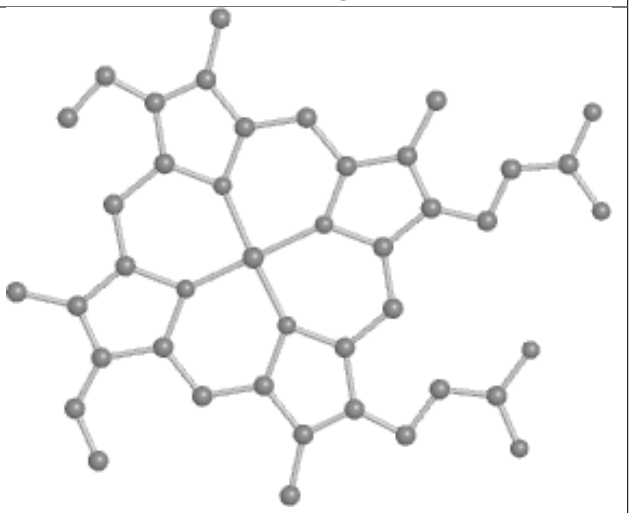
Bond lengths



Bond angles

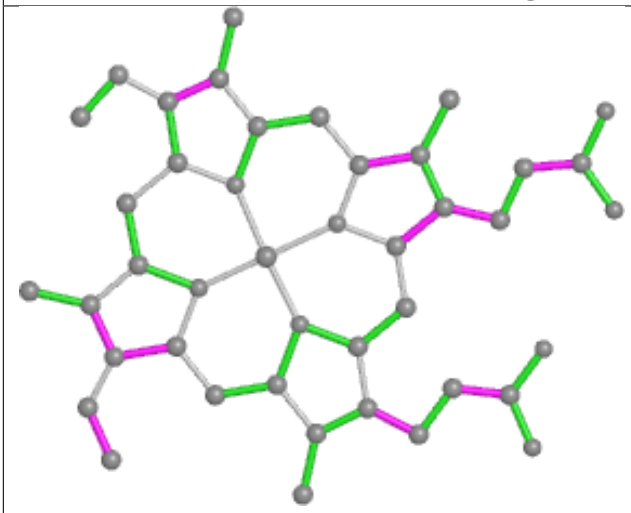


Torsions

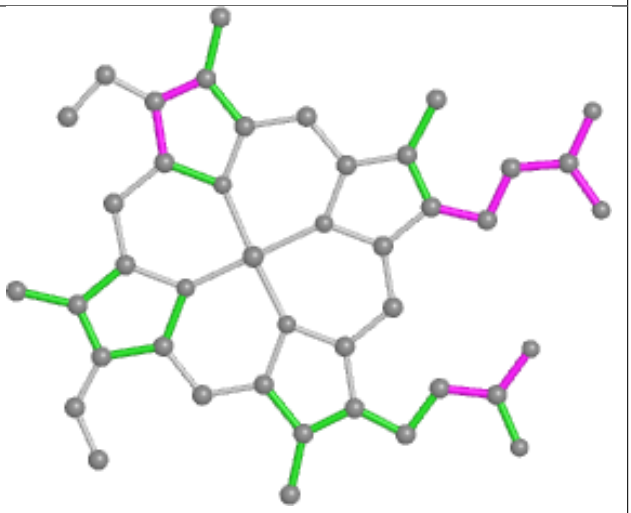


Rings

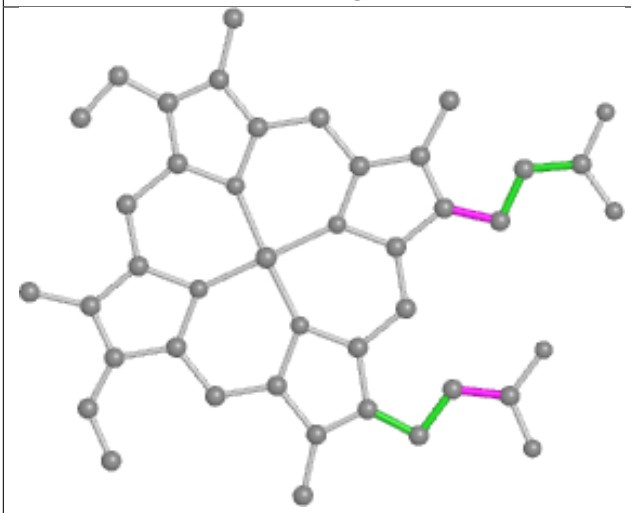
Ligand HEC D 242



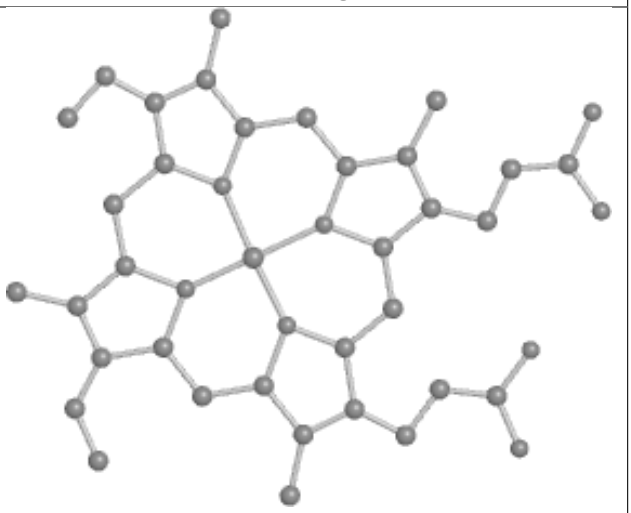
Bond lengths



Bond angles

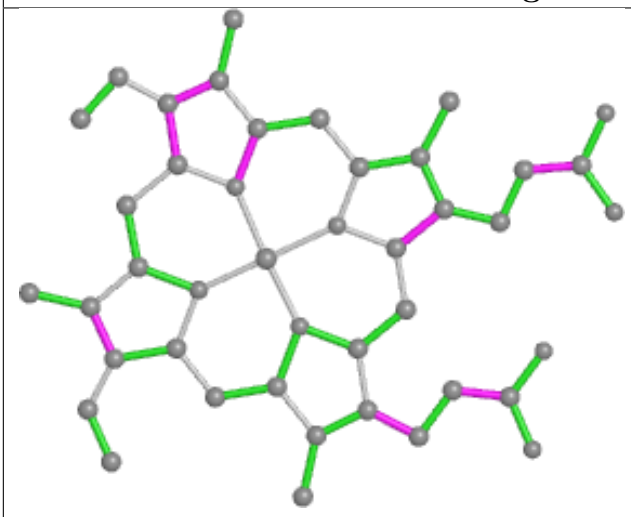


Torsions

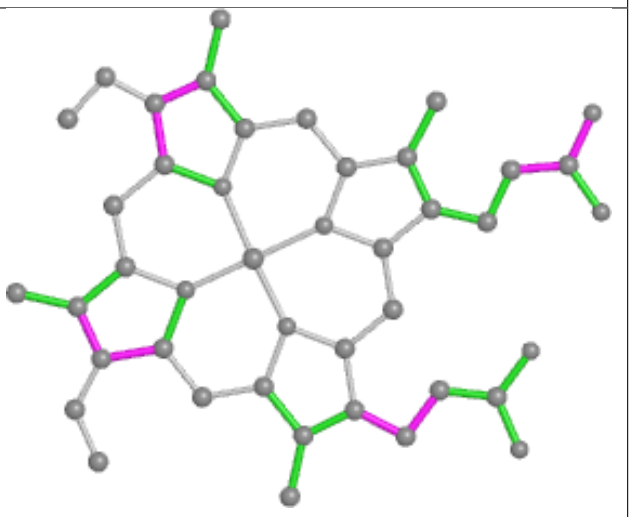


Rings

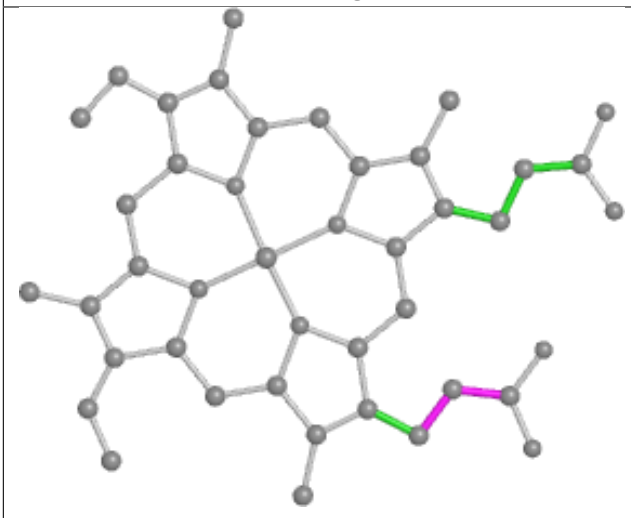
Ligand HEC C 381



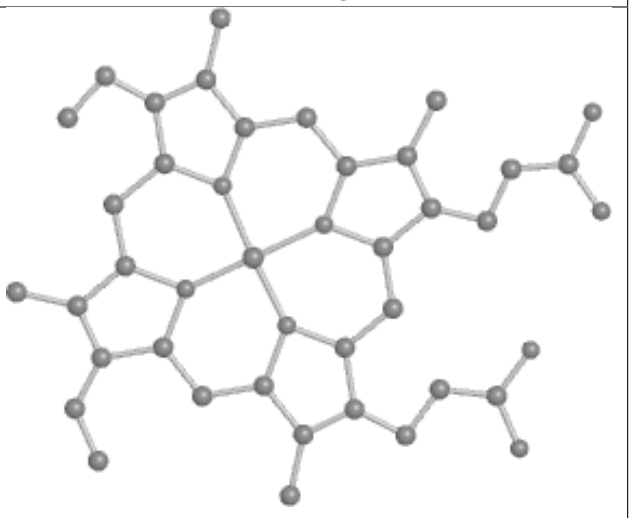
Bond lengths



Bond angles



Torsions



Rings

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.