



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 12:48 PM EDT

PDB ID : 1SQQ / pdb_00001sqq
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

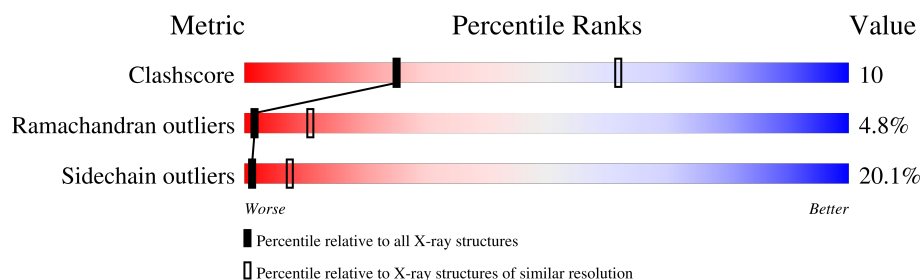
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

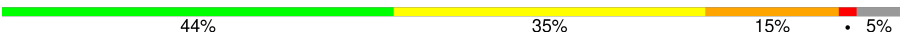
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	446	63% 27% 9% .
2	B	439	65% 23% 7% . .
3	C	379	57% 34% 7% .
4	D	241	49% 35% 12% 5%
5	E	196	70% 22% 6% .
6	F	110	58% 31% . . 5%
7	G	81	51% 31% 6% 5% 7%
8	H	78	35% 37% 14% . 10%

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	HEC	C	381	X	-	-	-

2 Entry composition

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
1	A	446	Total	C	N	O	S	0	0	0
			3458	2161	609	668	20			

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

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

- Molecule 3 is a protein called Cytochrome b.

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

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

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

- Molecule 5 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial 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
5	E	196	Total	C	N	O	S	0	0	0
			1519	957	263	291	8			

- 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			

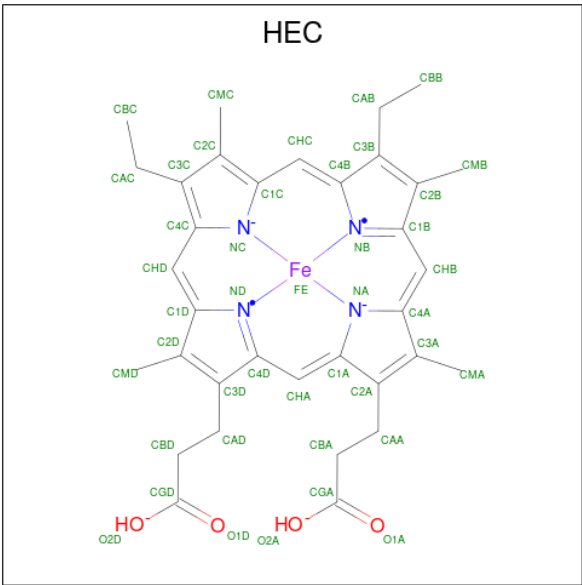
- Molecule 10 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

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.

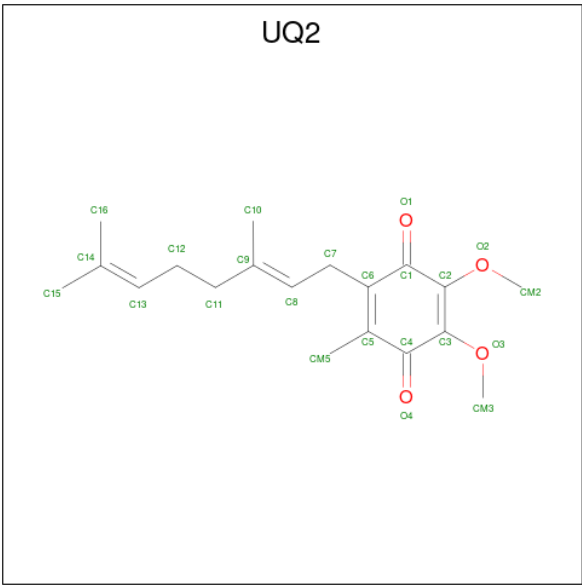
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	54	Total	C	N	O	S	0	0	0
			447	299	80	67	1			

- Molecule 12 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



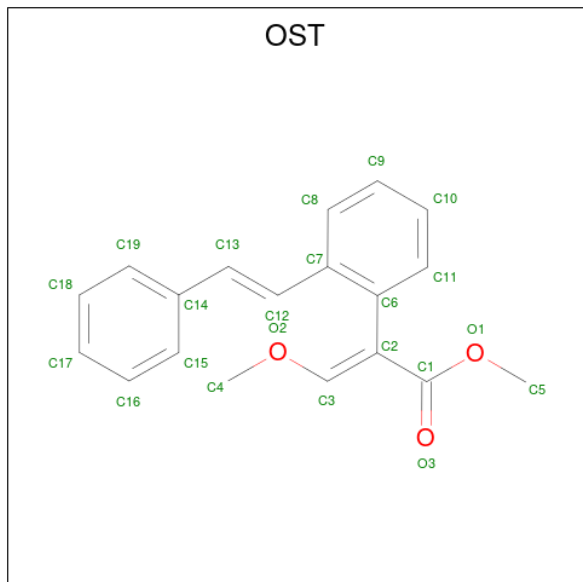
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 13 is UBIQUINONE-2 (CCD ID: UQ2) (formula: C₁₉H₂₆O₄).



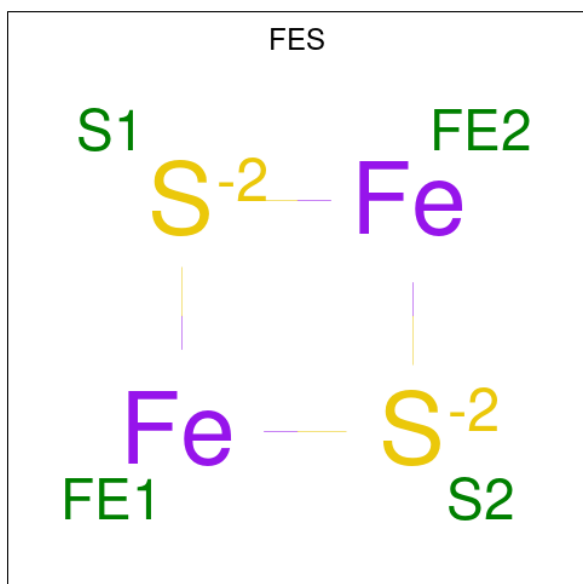
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	O	0	0
			23	19	4		

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



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

- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 16 is water.

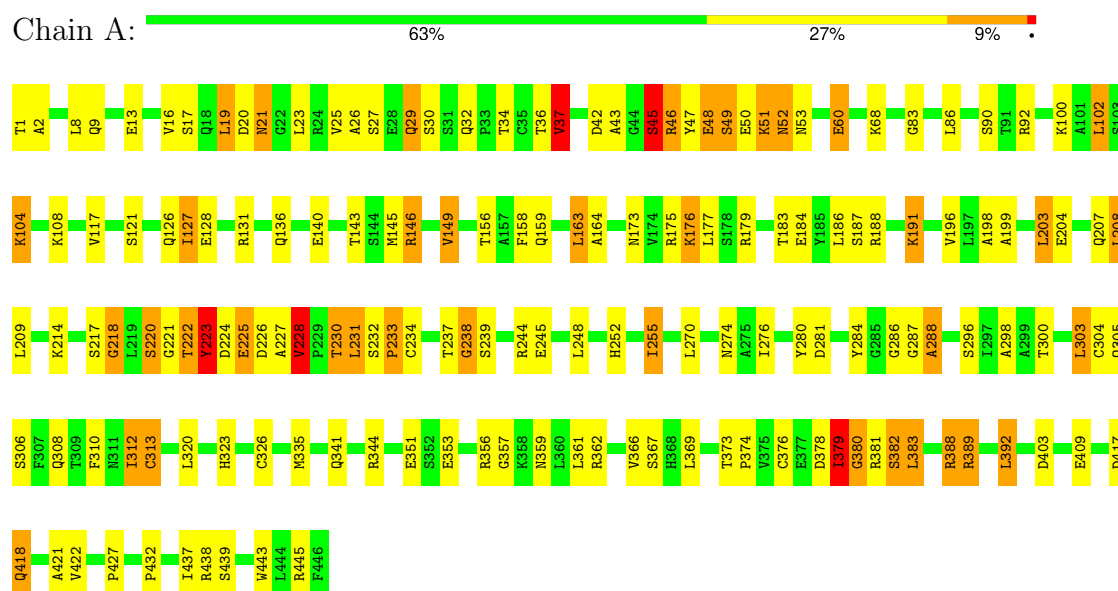
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	31	Total 31	O 31	0	0
16	B	78	Total 78	O 78	0	0
16	C	21	Total 21	O 21	0	0
16	D	5	Total 5	O 5	0	0
16	E	1	Total 1	O 1	0	0
16	F	25	Total 25	O 25	0	0
16	G	12	Total 12	O 12	0	0
16	H	2	Total 2	O 2	0	0
16	I	4	Total 4	O 4	0	0
16	J	1	Total 1	O 1	0	0
16	K	2	Total 2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

3 Residue-property plots

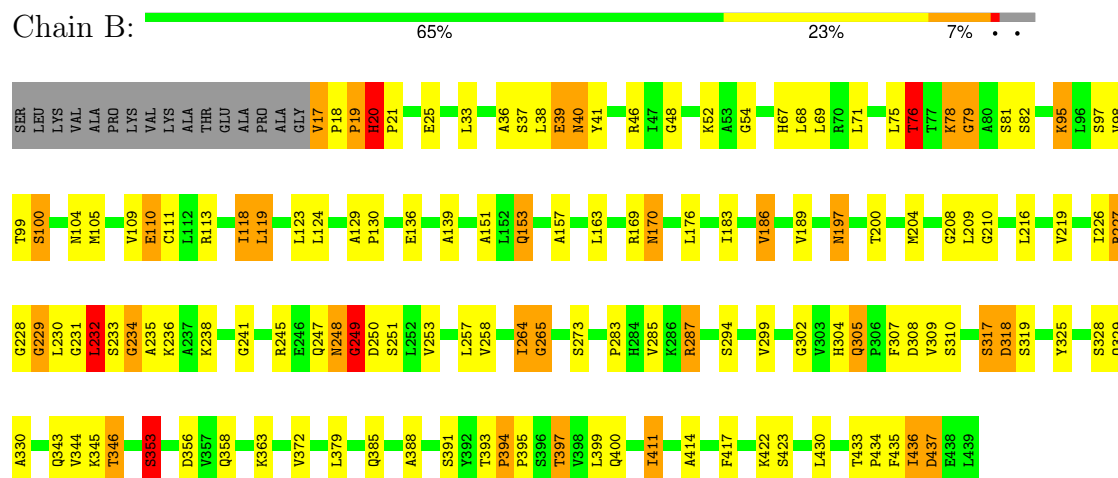
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

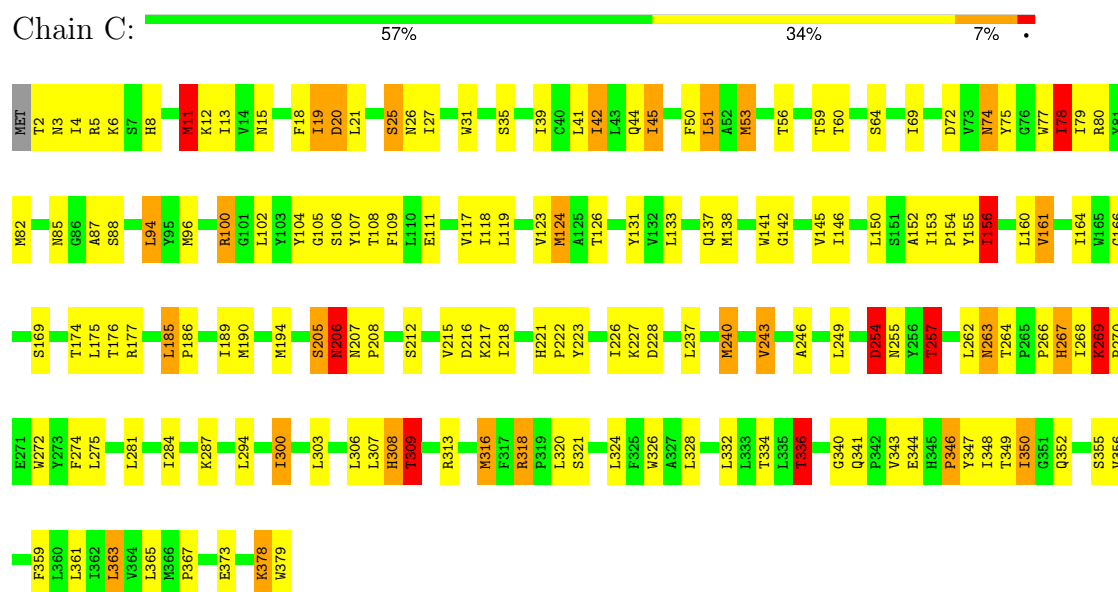
- Molecule 1: Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial precursor



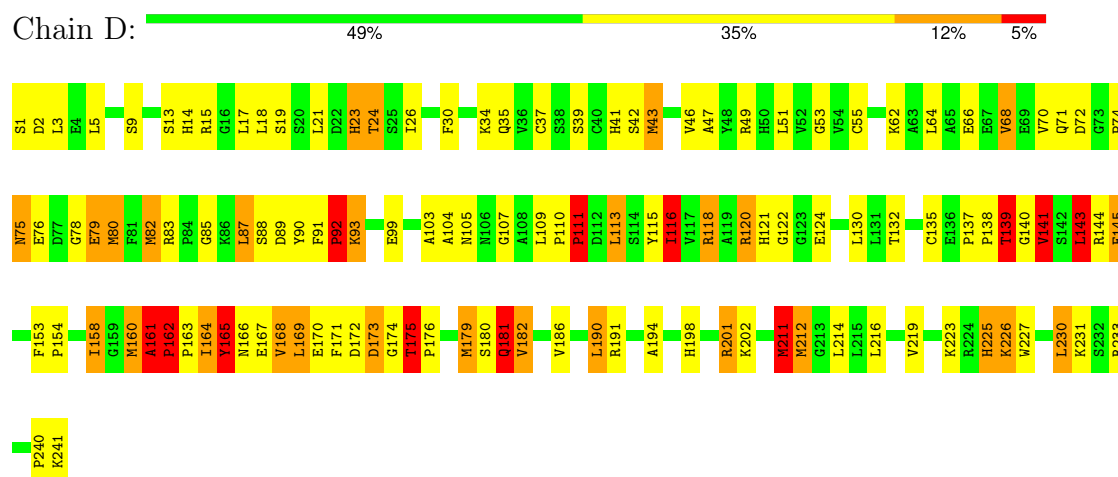
- Molecule 2: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial precursor



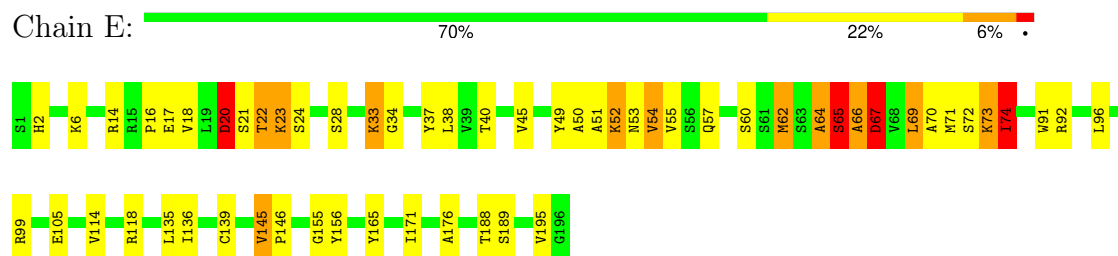
- Molecule 3: Cytochrome b



- Molecule 4: Cytochrome c1, heme protein, mitochondrial

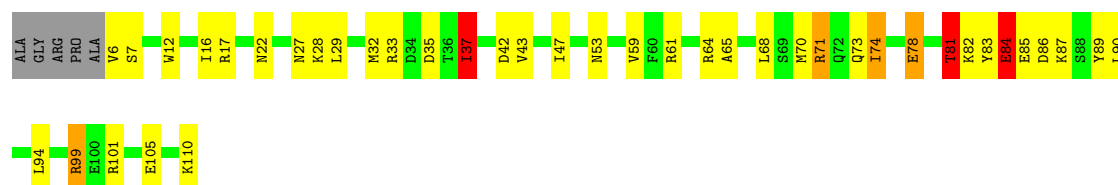


- Molecule 5: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial precursor (EC 1.10.2.2) (Rieske iron-sulfur protein) (RISP) [Contains: Ubiquinol-cytochrome c reductase 8 kDa protein (Complex III subunit IX)]



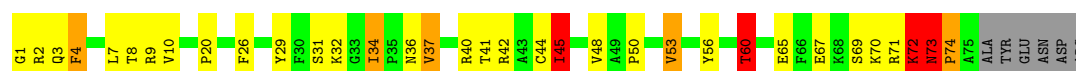
- Molecule 6: Ubiquinol-cytochrome c reductase complex 14 kDa protein

Chain F: 



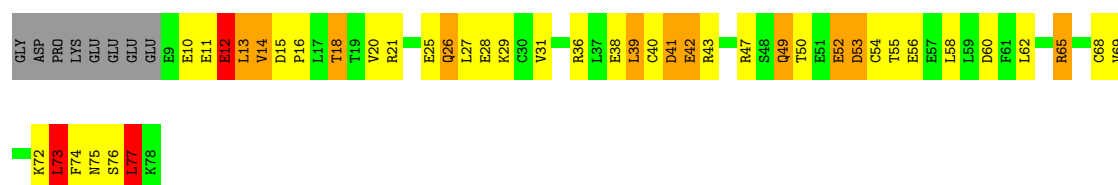
- Molecule 7: Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C

Chain G: 



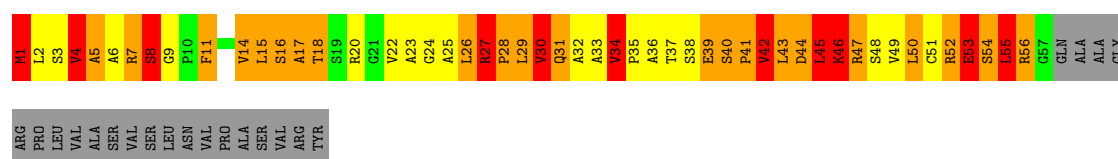
- Molecule 8: Ubiquinol-cytochrome c reductase complex 11 kDa protein

Chain H: 



- 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)]

Chain I: 



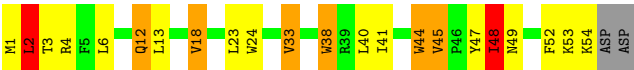
- Molecule 10: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

Chain J: 



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

Chain K: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OST, UQ2, FES, 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	1.18	6/3531 (0.2%)	1.10	2/4792 (0.0%)
2	B	1.38	13/3232 (0.4%)	1.17	4/4386 (0.1%)
3	C	1.28	16/3100 (0.5%)	1.21	8/4242 (0.2%)
4	D	1.24	11/1977 (0.6%)	1.12	7/2684 (0.3%)
5	E	0.90	3/1553 (0.2%)	1.08	7/2100 (0.3%)
6	F	1.26	4/930 (0.4%)	1.18	0/1246
7	G	1.56	7/649 (1.1%)	1.25	4/878 (0.5%)
8	H	1.27	3/580 (0.5%)	1.18	0/777
9	I	2.16	15/411 (3.6%)	1.53	8/558 (1.4%)
10	J	1.32	6/503 (1.2%)	1.18	1/678 (0.1%)
11	K	1.32	5/463 (1.1%)	1.12	0/632
All	All	1.29	89/16929 (0.5%)	1.16	41/22973 (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 (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	34	ILE	CA-CB	19.05	1.63	1.54
4	D	211	MET	SD-CE	-10.77	1.52	1.79
3	C	124	MET	SD-CE	9.56	2.03	1.79
3	C	240	MET	SD-CE	-8.62	1.57	1.79
9	I	46	LYS	CA-C	8.62	1.61	1.53
9	I	42	VAL	CA-CB	8.59	1.66	1.54
3	C	257	THR	CA-CB	8.18	1.66	1.53
9	I	4	VAL	CA-CB	8.16	1.64	1.54
1	A	288	ALA	CA-CB	-8.00	1.40	1.53
3	C	336	THR	CA-CB	7.88	1.65	1.53
7	G	53	VAL	CA-CB	7.87	1.64	1.54
9	I	26	LEU	CA-C	7.75	1.62	1.53
4	D	158	ILE	CA-CB	7.21	1.63	1.54
1	A	127	ILE	CA-CB	7.17	1.65	1.54
3	C	11	MET	SD-CE	7.09	1.97	1.79
2	B	411	ILE	CA-CB	7.06	1.62	1.54
3	C	42	ILE	CA-CB	7.03	1.63	1.54
2	B	105	MET	SD-CE	-6.96	1.62	1.79
4	D	162	PRO	CA-C	6.94	1.58	1.52
6	F	81	THR	CA-CB	6.94	1.63	1.53
9	I	53	GLU	CA-C	6.88	1.61	1.52
2	B	226	ILE	CA-CB	6.70	1.62	1.53
1	A	421	ALA	CA-CB	-6.70	1.43	1.53
11	K	18	VAL	CA-CB	6.63	1.62	1.54
2	B	151	ALA	CA-CB	-6.59	1.43	1.53
3	C	69	ILE	CA-CB	6.55	1.61	1.54
10	J	46	ILE	CA-CB	6.47	1.62	1.54
3	C	348	ILE	CA-CB	6.44	1.61	1.54
2	B	139	ALA	CA-CB	-6.43	1.42	1.53
4	D	116	ILE	CA-CB	6.42	1.63	1.54
3	C	156	ILE	CA-CB	6.42	1.63	1.54
9	I	45	LEU	CA-C	6.36	1.61	1.52
3	C	138	MET	SD-CE	-6.27	1.63	1.79
8	H	14	VAL	CA-CB	6.23	1.61	1.53
11	K	45	VAL	CA-C	6.22	1.58	1.53
10	J	4	THR	CA-CB	6.20	1.61	1.52
10	J	24	ILE	CA-CB	6.20	1.62	1.54
3	C	350	ILE	CA-CB	6.19	1.61	1.54
9	I	54	SER	N-CA	6.14	1.54	1.46
8	H	69	VAL	CA-CB	6.10	1.61	1.54
11	K	33	VAL	CA-CB	6.08	1.61	1.54
3	C	13	ILE	CA-CB	6.04	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	356	VAL	CA-CB	5.92	1.60	1.54
2	B	118	ILE	CA-CB	5.90	1.62	1.54
9	I	17	ALA	CA-C	5.87	1.61	1.52
4	D	182	VAL	CA-CB	5.85	1.62	1.54
8	H	31	VAL	CA-CB	5.82	1.61	1.54
9	I	54	SER	CA-C	5.81	1.60	1.52
11	K	48	ILE	CA-CB	5.73	1.63	1.54
3	C	316	MET	SD-CE	-5.68	1.65	1.79
7	G	73	ASN	CA-C	5.66	1.59	1.52
7	G	10	VAL	CA-CB	5.65	1.62	1.54
2	B	67	HIS	CA-C	-5.65	1.45	1.52
6	F	16	ILE	CA-CB	5.64	1.61	1.54
2	B	394	PRO	CA-C	5.63	1.57	1.52
5	E	62	MET	SD-CE	-5.63	1.65	1.79
2	B	414	ALA	CA-CB	-5.58	1.44	1.53
2	B	299	VAL	CA-CB	5.57	1.61	1.54
4	D	168	VAL	CA-CB	5.56	1.62	1.54
4	D	175	THR	CA-C	5.51	1.59	1.52
7	G	9	ARG	C-O	-5.51	1.17	1.23
4	D	43	MET	SD-CE	5.46	1.93	1.79
4	D	82	MET	SD-CE	5.40	1.93	1.79
9	I	43	LEU	N-CA	5.37	1.53	1.46
3	C	118	ILE	CA-CB	5.35	1.60	1.54
1	A	230	THR	CA-CB	5.33	1.60	1.53
7	G	37	VAL	CA-CB	5.33	1.61	1.54
7	G	2	ARG	N-CA	5.32	1.53	1.46
2	B	249	GLY	CA-C	5.31	1.59	1.51
1	A	335	MET	SD-CE	-5.29	1.66	1.79
4	D	212	MET	SD-CE	-5.29	1.66	1.79
9	I	46	LYS	N-CA	5.29	1.51	1.46
5	E	65	SER	CA-C	-5.29	1.45	1.52
10	J	51	LEU	CA-C	5.28	1.59	1.52
9	I	34	VAL	CA-CB	5.26	1.60	1.54
9	I	30	VAL	CA-CB	5.25	1.60	1.54
5	E	40	THR	CA-CB	5.23	1.61	1.53
11	K	2	LEU	CA-C	5.21	1.59	1.52
6	F	37	ILE	CA-CB	5.20	1.60	1.54
9	I	42	VAL	CA-C	5.20	1.59	1.52
3	C	309	THR	N-CA	5.19	1.52	1.46
10	J	42	ILE	CA-CB	5.14	1.61	1.54
2	B	48	GLY	CA-C	-5.13	1.48	1.52
9	I	45	LEU	N-CA	5.13	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	219	VAL	CA-CB	5.12	1.60	1.54
1	A	228	VAL	CA-CB	5.11	1.60	1.54
6	F	32	MET	SD-CE	5.09	1.92	1.79
10	J	55	ILE	CA-CB	5.08	1.61	1.54
2	B	100	SER	CA-C	5.07	1.59	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	226	ILE	N-CA-C	8.53	118.55	110.53
5	E	114	VAL	N-CA-C	8.31	119.09	110.62
7	G	34	ILE	N-CA-CB	8.23	116.03	110.52
2	B	197	ASN	N-CA-C	8.14	123.33	113.23
7	G	50	PRO	N-CA-C	7.56	119.92	110.70
5	E	2	HIS	N-CA-C	-7.31	104.35	113.20
9	I	26	LEU	N-CA-C	7.00	122.25	108.18
4	D	120	ARG	N-CA-C	6.82	121.38	111.02
9	I	27	ARG	N-CA-C	6.58	124.34	109.81
3	C	318	ARG	N-CA-C	6.48	122.84	108.27
1	A	26	ALA	N-CA-C	6.41	119.17	109.23
4	D	92	PRO	N-CA-C	6.41	125.67	112.47
9	I	55	LEU	N-CA-C	6.40	115.86	108.49
5	E	23	LYS	N-CA-C	6.39	119.94	109.72
5	E	20	ASP	N-CA-C	6.22	118.83	108.20
2	B	372	VAL	N-CA-C	6.07	118.00	112.29
7	G	60	THR	N-CA-C	6.00	117.90	111.36
3	C	308	HIS	N-CA-C	5.84	117.44	111.14
9	I	11	PHE	N-CA-C	5.83	119.41	110.20
10	J	24	ILE	N-CA-C	5.76	116.49	110.62
9	I	46	LYS	N-CA-C	5.72	115.06	108.49
9	I	52	ARG	N-CA-C	5.58	117.75	108.99
3	C	133	LEU	N-CA-C	5.53	120.44	113.25
4	D	175	THR	N-CA-C	5.51	121.99	109.81
9	I	42	VAL	CB-CA-C	5.49	120.29	111.29
1	A	326	CYS	N-CA-C	5.46	116.57	108.60
4	D	141	VAL	N-CA-C	5.45	115.42	108.12
3	C	19	ILE	N-CA-C	5.44	116.83	111.67
3	C	78	ILE	N-CA-CB	5.42	116.89	110.55
4	D	115	TYR	N-CA-C	5.39	119.55	112.92
9	I	45	LEU	N-CA-C	5.39	122.28	110.80
2	B	76	THR	N-CA-CB	5.31	117.77	109.85
5	E	145	VAL	N-CA-C	5.30	113.70	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	355	SER	N-CA-C	5.30	117.48	111.02
5	E	6	LYS	N-CA-C	-5.27	101.97	110.14
3	C	269	LYS	CB-CA-C	5.27	115.85	109.85
5	E	33	LYS	N-CA-C	-5.23	105.49	111.14
7	G	45	ILE	N-CA-CB	5.17	116.25	110.51
4	D	91	PHE	N-CA-C	5.16	121.22	109.81
2	B	100	SER	N-CA-C	5.06	117.77	110.28
4	D	230	LEU	N-CA-C	5.03	116.45	111.07

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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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

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	68	0
2	B	3172	0	3152	56	0
3	C	3003	0	3065	82	0
4	D	1918	0	1870	41	0
5	E	1519	0	1502	61	0
6	F	911	0	904	17	0
7	G	628	0	636	11	0
8	H	575	0	548	10	0
9	I	406	0	437	30	0
10	J	490	0	489	8	0
11	K	447	0	460	2	0
12	C	86	0	64	11	0
12	D	43	0	32	4	0
13	C	23	0	26	6	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	323	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 10.

All (323) 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
3:C:53:MET:HE1	5:E:62:MET:HG2	1.37	1.05
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
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
2:B:247:GLN:HE22	2:B:430:LEU:H	1.37	0.72
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
3:C:53:MET:SD	5:E:62:MET:HE2	2.30	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
2:B:283:PRO:HG3	9:I:31:GLN:HG3	1.76	0.66
3:C:228:ASP:OD2	13:C:383:UQ2:H5M3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:GLN:NE2	9:I:46:LYS:HG3	2.11	0.66
3:C:53:MET:HE1	5:E:62:MET:CG	2.20	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
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
5:E:70:ALA:C	5:E:72:SER:H	2.09	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
3:C:53:MET:CE	5:E:62:MET:HG2	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:50:PHE:CE2	5:E:62:MET:HE3	2.39	0.57
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
5:E:65:SER:O	5:E:66:ALA:C	2.48	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: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
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
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
3:C:35:SER:HB3	13:C:383:UQ2:CM5	2.37	0.54
3:C:35:SER:HB3	13:C:383:UQ2:H5M2	1.90	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
5:E:65:SER:C	5:E:67:ASP:N	2.65	0.53
9:I:42:VAL:HA	9:I:46:LYS:HZ2	1.74	0.53
4:D:211:MET:HE1	10:J:31:PHE:CE2	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:27:ILE:HD11	13:C:383:UQ2:H3M1	1.91	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
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
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
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
4:D:231:LYS:HD3	6:F:70:MET:HE3	1.94	0.50
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
3:C:237:LEU:HA	4:D:212:MET:HE3	1.94	0.49
4:D:37:CYS:SG	12:D:242:HEC:CAB	2.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:F:28:LYS:HB3	6:F:74:ILE:CG1	2.44	0.48
7:G:3:GLN:O	7:G:4:PHE:HB2	2.11	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
4:D:160:MET:HE3	4:D:163:PRO:HD3	1.96	0.47
1:A:373:THR:HB	1:A:374:PRO:HD3	1.96	0.47
4:D:211:MET:HE1	10:J:31:PHE:HE2	1.79	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:52:LYS:O	5:E:53:ASN:C	2.56	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
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
5:E:16:PRO:C	5:E:18:VAL:H	2.23	0.47
3:C:78:ILE:HB	3:C:82:MET:HE3	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
6:F:82:LYS:C	6:F:84:GLU:O	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:C:53:MET:HE1	5:E:62:MET:HE2	1.98	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
3:C:82:MET:HG2	3:C:240:MET:HE1	1.98	0.45
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:70:ALA:C	5:E:72:SER:N	2.74	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
5:E:33:LYS:O	5:E:34:GLY:C	2.60	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:35:ASP:OD2	6:F:89:TYR:OH	2.32	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
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
5:E:20:ASP:CG	5:E:22:THR:HG23	2.43	0.44
1:A:45:SER:C	1:A:47:TYR:H	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:E:49:TYR:CD2	5:E:49:TYR:C	2.97	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: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
4:D:211:MET:HE2	10:J:35:PHE:CE2	2.54	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
4:D:211:MET:HE3	5:E:49:TYR:CD2	2.54	0.42
9:I:1:MET:O	9:I:1:MET:HE2	2.19	0.42
1:A:45:SER:C	1:A:47:TYR:N	2.78	0.42
1:A:255:ILE:HD12	1:A:422:VAL:HG22	2.00	0.42
3:C:80:ARG:C	3:C:80:ARG:HD3	2.45	0.42
3:C:131:TYR:HA	12:C:381:HEC:HAD2	2.01	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
3:C:217:LYS:HG3	7:G:7:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:36:THR:O	1:A:199:ALA:HA	2.20	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
3:C:53:MET:CE	5:E:62:MET:HE2	2.50	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
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
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
4:D:90:TYR:C	4:D:92:PRO:HD2	2.47	0.40
5:E:37:TYR:O	5:E:38:LEU:C	2.65	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
5:E:16:PRO:C	5:E:18:VAL:N	2.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	444/446 (100%)	393 (88%)	34 (8%)	17 (4%)	2	15
2	B	421/439 (96%)	377 (90%)	31 (7%)	13 (3%)	3	19
3	C	376/379 (99%)	321 (85%)	41 (11%)	14 (4%)	2	15
4	D	239/241 (99%)	187 (78%)	33 (14%)	19 (8%)	1	3
5	E	194/196 (99%)	174 (90%)	12 (6%)	8 (4%)	2	13
6	F	103/110 (94%)	91 (88%)	10 (10%)	2 (2%)	6	30
7	G	73/81 (90%)	66 (90%)	4 (6%)	3 (4%)	2	13
8	H	68/78 (87%)	56 (82%)	7 (10%)	5 (7%)	1	4
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%)	2	15
All	All	2082/2166 (96%)	1779 (85%)	203 (10%)	100 (5%)	2	11

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
2	B	232	LEU
2	B	250	ASP
2	B	305	GLN

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Mol	Chain	Res	Type
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
2	B	54	GLY
2	B	79	GLY
2	B	249	GLY

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Mol	Chain	Res	Type
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
4	D	170	GLU
10	J	36	ASP
1	A	233	PRO

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Mol	Chain	Res	Type
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%)	296 (80%)	74 (20%)	1	7
2	B	332/343 (97%)	285 (86%)	47 (14%)	3	16
3	C	326/327 (100%)	264 (81%)	62 (19%)	1	8
4	D	206/206 (100%)	153 (74%)	53 (26%)	0	3
5	E	168/168 (100%)	156 (93%)	12 (7%)	13	43
6	F	96/98 (98%)	76 (79%)	20 (21%)	1	7
7	G	66/71 (93%)	52 (79%)	14 (21%)	1	6
8	H	67/74 (90%)	45 (67%)	22 (33%)	0	1
9	I	44/60 (73%)	21 (48%)	23 (52%)	0	0
10	J	50/52 (96%)	36 (72%)	14 (28%)	0	2
11	K	44/46 (96%)	30 (68%)	14 (32%)	0	1
All	All	1769/1815 (98%)	1414 (80%)	355 (20%)	1	7

All (355) 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	16	VAL
1	A	17	SER
1	A	19	LEU
1	A	23	LEU
1	A	29	GLN

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Mol	Chain	Res	Type
1	A	32	GLN
1	A	34	THR
1	A	37	VAL
1	A	48	GLU
1	A	51	LYS
1	A	52	ASN
1	A	60	GLU
1	A	68	LYS
1	A	90	SER
1	A	100	LYS
1	A	102	LEU
1	A	104	LYS
1	A	108	LYS
1	A	117	VAL
1	A	126	GLN
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	149	VAL
1	A	163	LEU
1	A	175	ARG
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	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

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Mol	Chain	Res	Type
1	A	228	VAL
1	A	230	THR
1	A	231	LEU
1	A	245	GLU
1	A	255	ILE
1	A	274	ASN
1	A	296	SER
1	A	300	THR
1	A	305	GLN
1	A	313	CYS
1	A	361	LEU
1	A	366	VAL
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	403	ASP
1	A	409	GLU
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	95	LYS
2	B	97	SER
2	B	98	VAL
2	B	104	ASN
2	B	109	VAL
2	B	110	GLU
2	B	118	ILE
2	B	119	LEU
2	B	123	LEU
2	B	163	LEU

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Mol	Chain	Res	Type
2	B	176	LEU
2	B	183	ILE
2	B	186	VAL
2	B	189	VAL
2	B	197	ASN
2	B	204	MET
2	B	209	LEU
2	B	227	ARG
2	B	230	LEU
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	287	ARG
2	B	294	SER
2	B	309	VAL
2	B	329	GLN
2	B	345	LYS
2	B	346	THR
2	B	353	SER
2	B	358	GLN
2	B	379	LEU
2	B	397	THR
2	B	411	ILE
2	B	422	LYS
2	B	435	PHE
2	B	437	ASP
3	C	2	THR
3	C	4	ILE
3	C	11	MET
3	C	18	PHE
3	C	25	SER
3	C	39	ILE
3	C	41	LEU
3	C	42	ILE
3	C	45	ILE
3	C	51	LEU
3	C	56	THR
3	C	59	THR
3	C	60	THR

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Mol	Chain	Res	Type
3	C	64	SER
3	C	74	ASN
3	C	78	ILE
3	C	88	SER
3	C	94	LEU
3	C	96	MET
3	C	100	ARG
3	C	102	LEU
3	C	111	GLU
3	C	145	VAL
3	C	156	ILE
3	C	160	LEU
3	C	161	VAL
3	C	164	ILE
3	C	174	THR
3	C	175	LEU
3	C	176	THR
3	C	185	LEU
3	C	190	MET
3	C	194	MET
3	C	205	SER
3	C	206	ASN
3	C	212	SER
3	C	215	VAL
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	281	LEU
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	316	MET
3	C	320	LEU
3	C	321	SER
3	C	324	LEU
3	C	328	LEU

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Mol	Chain	Res	Type
3	C	334	THR
3	C	336	THR
3	C	341	GLN
3	C	350	ILE
3	C	363	LEU
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	35	GLN
4	D	39	SER
4	D	42	SER
4	D	43	MET
4	D	46	VAL
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	87	LEU
4	D	99	GLU
4	D	113	LEU
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

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Mol	Chain	Res	Type
4	D	143	LEU
4	D	145	GLU
4	D	158	ILE
4	D	165	TYR
4	D	168	VAL
4	D	169	LEU
4	D	173	ASP
4	D	179	MET
4	D	181	GLN
4	D	186	VAL
4	D	190	LEU
4	D	201	ARG
4	D	211	MET
4	D	214	LEU
4	D	223	LYS
4	D	225	HIS
4	D	226	LYS
4	D	241	LYS
5	E	20	ASP
5	E	21	SER
5	E	22	THR
5	E	52	LYS
5	E	54	VAL
5	E	60	SER
5	E	65	SER
5	E	67	ASP
5	E	74	ILE
5	E	135	LEU
5	E	188	THR
5	E	189	SER
6	F	7	SER
6	F	12	TRP
6	F	22	ASN
6	F	29	LEU
6	F	33	ARG
6	F	37	ILE
6	F	53	ASN
6	F	59	VAL
6	F	64	ARG
6	F	71	ARG
6	F	73	GLN
6	F	74	ILE

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Mol	Chain	Res	Type
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	32	LYS
7	G	34	ILE
7	G	36	ASN
7	G	37	VAL
7	G	40	ARG
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
8	H	14	VAL
8	H	18	THR
8	H	20	VAL
8	H	29	LYS
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

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Mol	Chain	Res	Type
8	H	72	LYS
8	H	77	LEU
9	I	1	MET
9	I	7	ARG
9	I	8	SER
9	I	14	VAL
9	I	15	LEU
9	I	16	SER
9	I	18	THR
9	I	22	VAL
9	I	27	ARG
9	I	30	VAL
9	I	31	GLN
9	I	34	VAL
9	I	37	THR
9	I	39	GLU
9	I	44	ASP
9	I	45	LEU
9	I	46	LYS
9	I	47	ARG
9	I	48	SER
9	I	50	LEU
9	I	53	GLU
9	I	55	LEU
9	I	56	ARG
10	J	4	THR
10	J	5	LEU
10	J	8	ARG
10	J	9	LEU
10	J	12	LEU
10	J	16	ARG
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

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Mol	Chain	Res	Type
11	K	12	GLN
11	K	13	LEU
11	K	18	VAL
11	K	23	LEU
11	K	24	TRP
11	K	38	TRP
11	K	40	LEU
11	K	44	TRP
11	K	48	ILE
11	K	52	PHE
11	K	54	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	69	ASN
1	A	119	ASN
1	A	141	ASN
1	A	173	ASN
1	A	252	HIS
1	A	274	ASN
1	A	308	GLN
1	A	323	HIS
1	A	341	GLN
1	A	359	ASN
1	A	418	GLN
2	B	40	ASN
2	B	143	GLN
2	B	153	GLN
2	B	162	ASN
2	B	170	ASN
2	B	174	ASN
2	B	222	GLN
2	B	247	GLN
2	B	248	ASN
2	B	276	GLN
2	B	277	HIS
2	B	284	HIS
2	B	329	GLN
2	B	342	ASN
2	B	343	GLN

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Mol	Chain	Res	Type
2	B	351	ASN
2	B	362	ASN
2	B	385	GLN
3	C	3	ASN
3	C	8	HIS
3	C	26	ASN
3	C	32	ASN
3	C	74	ASN
3	C	85	ASN
3	C	114	ASN
3	C	137	GLN
3	C	201	HIS
3	C	206	ASN
3	C	267	HIS
3	C	322	GLN
3	C	352	GLN
4	D	97	ASN
4	D	105	ASN
4	D	181	GLN
4	D	200	HIS
4	D	225	HIS
5	E	57	GLN
5	E	161	HIS
6	F	73	GLN
7	G	6	HIS
7	G	73	ASN
8	H	75	ASN
10	J	61	ASN
11	K	12	GLN
11	K	16	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
12	HEC	C	381	3	50,50,50	1.38	5 (10%)	68,82,82	2.00	20 (29%)
12	HEC	C	382	3	50,50,50	1.53	9 (18%)	68,82,82	2.09	19 (27%)
12	HEC	D	242	4	50,50,50	1.33	7 (14%)	68,82,82	1.94	20 (29%)
14	OST	C	384	-	23,23,23	2.29	12 (52%)	29,29,29	1.46	6 (20%)
13	UQ2	C	383	-	23,23,23	2.90	8 (34%)	30,31,31	1.34	5 (16%)
15	FES	E	197	5	0,4,4	-	-	-	-	-

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	HEC	C	381	3	1/1/3/7	3/14/54/54	-
12	HEC	C	382	3	-	13/14/54/54	-
12	HEC	D	242	4	-	4/14/54/54	-
14	OST	C	384	-	-	6/18/18/18	0/2/2/2
13	UQ2	C	383	-	-	6/15/39/39	0/1/1/1
15	FES	E	197	5	-	-	0/1/1/1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	383	UQ2	C6-C5	8.98	1.51	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	383	UQ2	C8-C9	5.06	1.44	1.33
12	C	382	HEC	CBA-CGA	-4.83	1.39	1.50
13	C	383	UQ2	C3-C2	4.80	1.53	1.36
14	C	384	OST	C6-C7	4.52	1.47	1.41
12	C	382	HEC	CBD-CGD	-4.49	1.40	1.50
14	C	384	OST	C11-C6	4.12	1.46	1.39
13	C	383	UQ2	C7-C8	3.97	1.56	1.50
12	C	381	HEC	CBD-CGD	-3.77	1.41	1.50
12	D	242	HEC	FE-NA	3.30	2.06	1.95
13	C	383	UQ2	C13-C14	3.00	1.41	1.32
12	C	381	HEC	CHD-C4C	3.00	1.46	1.39
13	C	383	UQ2	C7-C6	2.99	1.57	1.51
12	D	242	HEC	CBD-CGD	-2.98	1.43	1.50
12	C	382	HEC	FE-ND	2.90	2.03	1.94
14	C	384	OST	C6-C2	2.88	1.52	1.49
14	C	384	OST	C16-C15	2.85	1.43	1.38
13	C	383	UQ2	C6-C1	2.85	1.54	1.46
14	C	384	OST	C15-C14	2.81	1.45	1.39
14	C	384	OST	O2-C3	-2.79	1.29	1.34
12	C	381	HEC	CBA-CGA	-2.79	1.44	1.50
14	C	384	OST	C17-C18	2.71	1.44	1.38
12	C	382	HEC	C4B-NB	-2.68	1.35	1.40
14	C	384	OST	C18-C19	2.65	1.43	1.38
13	C	383	UQ2	O2-C2	2.63	1.43	1.36
14	C	384	OST	C10-C11	2.62	1.43	1.38
12	C	382	HEC	CHD-C4C	2.58	1.45	1.39
12	D	242	HEC	CHD-C4C	2.58	1.45	1.39
12	C	381	HEC	FE-NA	2.57	2.03	1.95
14	C	384	OST	C17-C16	2.56	1.43	1.38
12	C	382	HEC	C4A-NA	-2.55	1.34	1.39
12	C	381	HEC	FE-NB	2.48	2.02	1.94
12	D	242	HEC	FE-NB	2.47	2.02	1.94
12	D	242	HEC	CBA-CGA	-2.28	1.45	1.50
12	C	382	HEC	O2D-CGD	-2.20	1.23	1.30
14	C	384	OST	C10-C9	2.15	1.43	1.38
12	C	382	HEC	O2A-CGA	-2.12	1.23	1.30
12	D	242	HEC	CAA-C2A	2.12	1.56	1.51
12	D	242	HEC	FE-ND	2.11	2.01	1.94
14	C	384	OST	C8-C7	2.02	1.44	1.41
12	C	382	HEC	FE-NA	2.01	2.01	1.95

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	381	HEC	CHB-C4A-NA	6.54	131.57	124.45
12	C	382	HEC	C2A-C1A-NA	-6.16	104.38	110.32
12	D	242	HEC	CHB-C4A-NA	5.50	130.44	124.45
12	D	242	HEC	CHA-C1A-NA	4.95	129.84	124.45
12	C	381	HEC	CHA-C1A-NA	4.73	129.60	124.45
12	C	382	HEC	CHB-C4A-NA	4.63	129.50	124.45
12	C	382	HEC	CHA-C1A-NA	4.61	129.48	124.45
12	C	381	HEC	C2A-C1A-NA	-4.44	106.04	110.32
12	C	382	HEC	C4A-CHB-C1B	-4.23	117.04	126.02
12	C	382	HEC	CAD-C3D-C4D	4.07	131.79	124.70
12	C	382	HEC	C4A-NA-C1A	4.04	112.40	105.82
12	C	382	HEC	CAD-C3D-C2D	-3.92	120.53	127.87
12	C	382	HEC	C4C-CHD-C1D	-3.83	117.24	126.25
12	D	242	HEC	CHC-C4B-NB	3.80	129.07	124.37
12	C	381	HEC	C4A-NA-C1A	3.56	111.62	105.82
12	D	242	HEC	CHB-C1B-NB	3.50	128.19	124.42
12	D	242	HEC	C2A-C1A-NA	-3.48	106.96	110.32
12	C	382	HEC	CAC-C3C-C2C	3.42	132.31	126.89
12	D	242	HEC	CHD-C1D-ND	3.40	128.58	124.37
12	C	381	HEC	CHD-C1D-ND	3.31	128.46	124.37
12	D	242	HEC	C4A-CHB-C1B	-3.31	118.98	126.02
12	C	381	HEC	CHB-C1B-NB	3.23	127.90	124.42
12	C	381	HEC	CHC-C4B-NB	3.22	128.36	124.37
12	C	381	HEC	C1C-CHC-C4B	-3.21	118.69	126.25
12	C	381	HEC	CHA-C4D-ND	3.19	127.85	124.42
12	C	382	HEC	CAA-C2A-C3A	-3.12	122.03	127.87
12	C	381	HEC	C4A-CHB-C1B	-3.09	119.44	126.02
12	C	381	HEC	C4C-CHD-C1D	-3.04	119.09	126.25
12	D	242	HEC	C4A-NA-C1A	2.96	110.65	105.82
12	C	382	HEC	CAA-C2A-C1A	2.95	130.85	124.85
12	C	382	HEC	CAC-C3C-C4C	-2.91	120.90	124.91
12	D	242	HEC	CHA-C4D-ND	2.88	127.52	124.42
13	C	383	UQ2	C7-C6-C5	-2.87	119.97	124.89
14	C	384	OST	C11-C6-C7	-2.83	115.81	119.29
12	D	242	HEC	C4C-CHD-C1D	-2.82	119.62	126.25
12	C	382	HEC	CHB-C1B-NB	2.82	127.46	124.42
12	C	381	HEC	CBB-CAB-C3B	-2.78	104.90	112.42
13	C	383	UQ2	C7-C6-C1	2.75	121.71	118.52
12	D	242	HEC	C1C-CHC-C4B	-2.73	119.82	126.25
12	D	242	HEC	CHC-C1C-NC	2.70	128.76	123.86
12	D	242	HEC	CBA-CAA-C2A	2.70	120.01	112.53
14	C	384	OST	O1-C1-C2	2.69	115.71	112.05
13	C	383	UQ2	C6-C5-C4	2.65	121.26	119.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	242	HEC	O2A-CGA-O1A	-2.63	116.56	123.33
12	C	382	HEC	O2A-CGA-CBA	2.63	122.30	114.00
14	C	384	OST	C3-C2-C1	-2.62	112.47	117.16
12	C	381	HEC	CHD-C4C-NC	2.55	128.49	123.86
13	C	383	UQ2	CM5-C5-C6	-2.55	120.26	124.45
12	C	382	HEC	C3A-C4A-NA	-2.54	104.94	109.64
12	C	382	HEC	C1C-CHC-C4B	-2.54	120.28	126.25
12	D	242	HEC	O2D-CGD-CBD	2.44	121.71	114.00
12	C	382	HEC	CHD-C1D-ND	2.35	127.28	124.37
12	D	242	HEC	CHD-C4C-NC	2.34	128.11	123.86
14	C	384	OST	C4-O2-C3	-2.28	111.91	115.65
12	C	382	HEC	CHC-C1C-NC	2.28	127.99	123.86
12	C	381	HEC	C1A-CHA-C4D	-2.27	121.19	126.02
12	D	242	HEC	C1A-CHA-C4D	-2.24	121.25	126.02
14	C	384	OST	C6-C2-C3	2.18	125.19	122.09
12	D	242	HEC	O2A-CGA-CBA	2.17	120.85	114.00
12	C	381	HEC	O2A-CGA-CBA	2.13	120.74	114.00
12	D	242	HEC	C3A-C4A-NA	-2.10	105.74	109.64
12	C	381	HEC	C3B-C4B-NB	-2.10	107.86	110.17
12	C	381	HEC	CHC-C1C-NC	2.10	127.67	123.86
12	C	381	HEC	CHA-C4D-C3D	-2.09	121.72	124.77
13	C	383	UQ2	C16-C14-C15	2.06	119.34	114.59
12	C	381	HEC	CHB-C1B-C2B	-2.06	121.78	125.03
12	C	382	HEC	CBC-CAC-C3C	2.05	117.98	112.42
12	C	381	HEC	O2D-CGD-CBD	2.03	120.41	114.00
14	C	384	OST	O1-C1-O3	-2.02	119.64	123.50
12	D	242	HEC	CAD-C3D-C4D	2.02	128.21	124.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	C	381	HEC	NA

All (32) 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
14	C	384	OST	O3-C1-C2-C3
14	C	384	OST	C1-C2-C3-O2
12	C	382	HEC	C2C-C3C-CAC-CBC
12	C	382	HEC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
12	C	382	HEC	C2D-C3D-CAD-CBD
12	C	382	HEC	C4D-C3D-CAD-CBD
13	C	383	UQ2	C9-C11-C12-C13
12	D	242	HEC	C1A-C2A-CAA-CBA
12	C	382	HEC	C4B-C3B-CAB-CBB
12	C	382	HEC	C2B-C3B-CAB-CBB
12	C	382	HEC	C3D-CAD-CBD-CGD
14	C	384	OST	O3-C1-C2-C6
13	C	383	UQ2	C12-C11-C9-C10
13	C	383	UQ2	C12-C11-C9-C8
12	C	381	HEC	C3D-CAD-CBD-CGD
13	C	383	UQ2	C1-C6-C7-C8
14	C	384	OST	O1-C1-C2-C3
12	D	242	HEC	C3A-C2A-CAA-CBA
14	C	384	OST	C12-C13-C14-C15
13	C	383	UQ2	C1-C2-O2-CM2
13	C	383	UQ2	C5-C6-C7-C8
12	C	381	HEC	CAD-CBD-CGD-O1D
12	D	242	HEC	CAD-CBD-CGD-O1D
12	C	382	HEC	CAD-CBD-CGD-O2D
12	D	242	HEC	CAD-CBD-CGD-O2D
12	C	381	HEC	CAD-CBD-CGD-O2D
12	C	382	HEC	CAD-CBD-CGD-O1D
12	C	382	HEC	CAA-CBA-CGA-O2A
12	C	382	HEC	CAA-CBA-CGA-O1A
14	C	384	OST	C12-C13-C14-C19

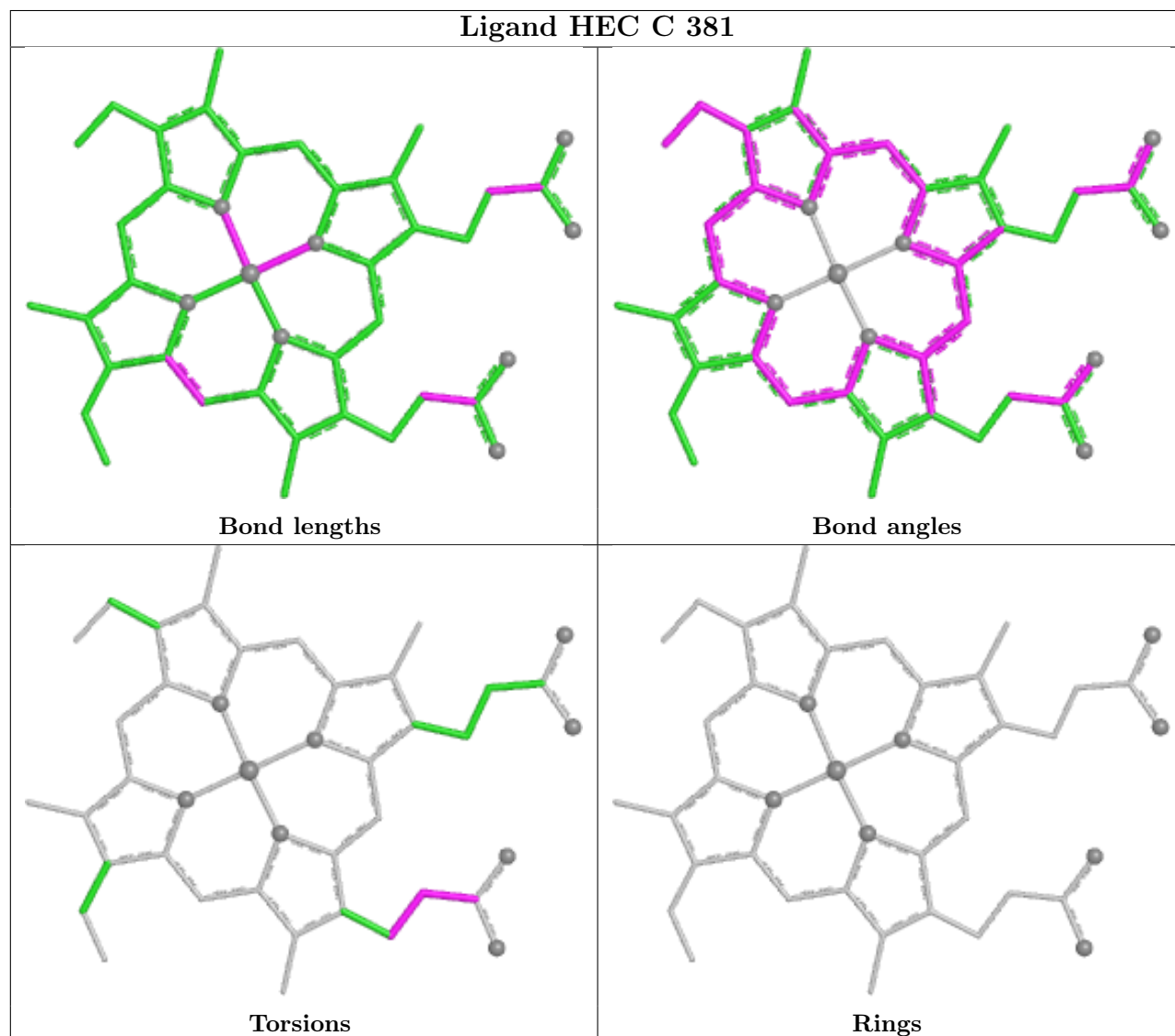
There are no ring outliers.

5 monomers are involved in 25 short contacts:

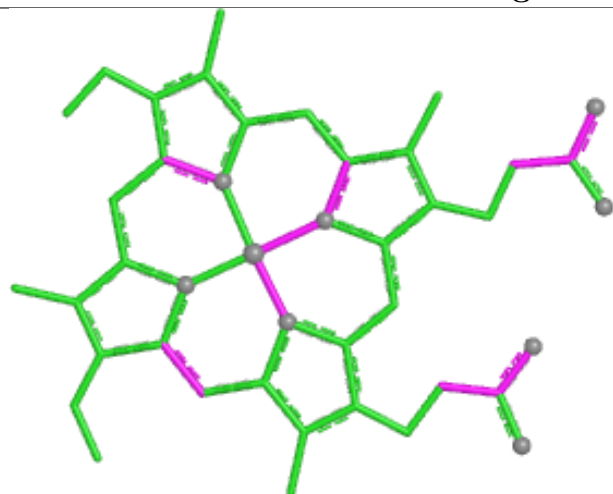
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	381	HEC	5	0
12	C	382	HEC	6	0
12	D	242	HEC	4	0
14	C	384	OST	4	0
13	C	383	UQ2	6	0

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 than 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.

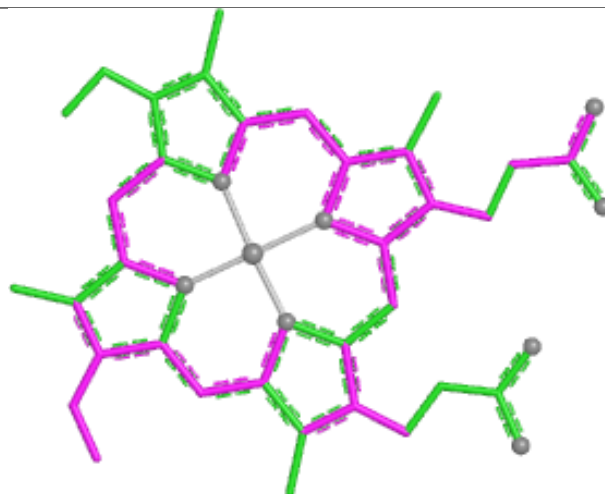
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



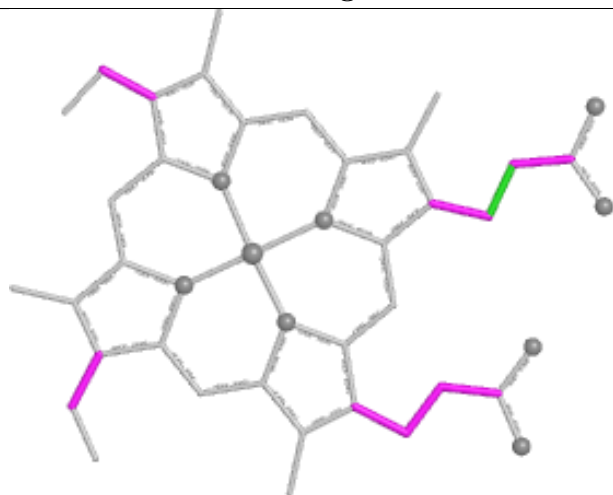
Ligand HEC C 382



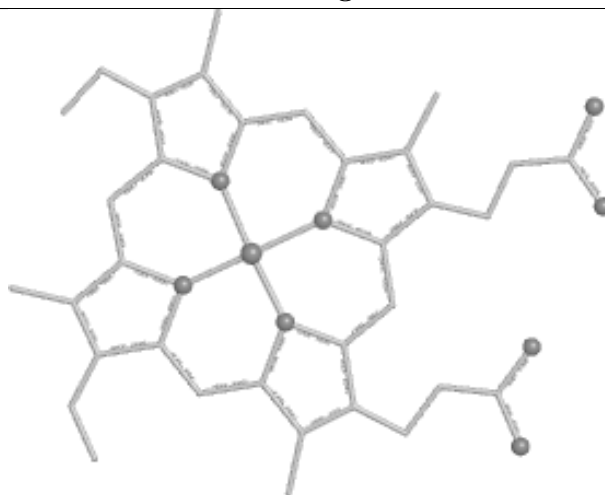
Bond lengths



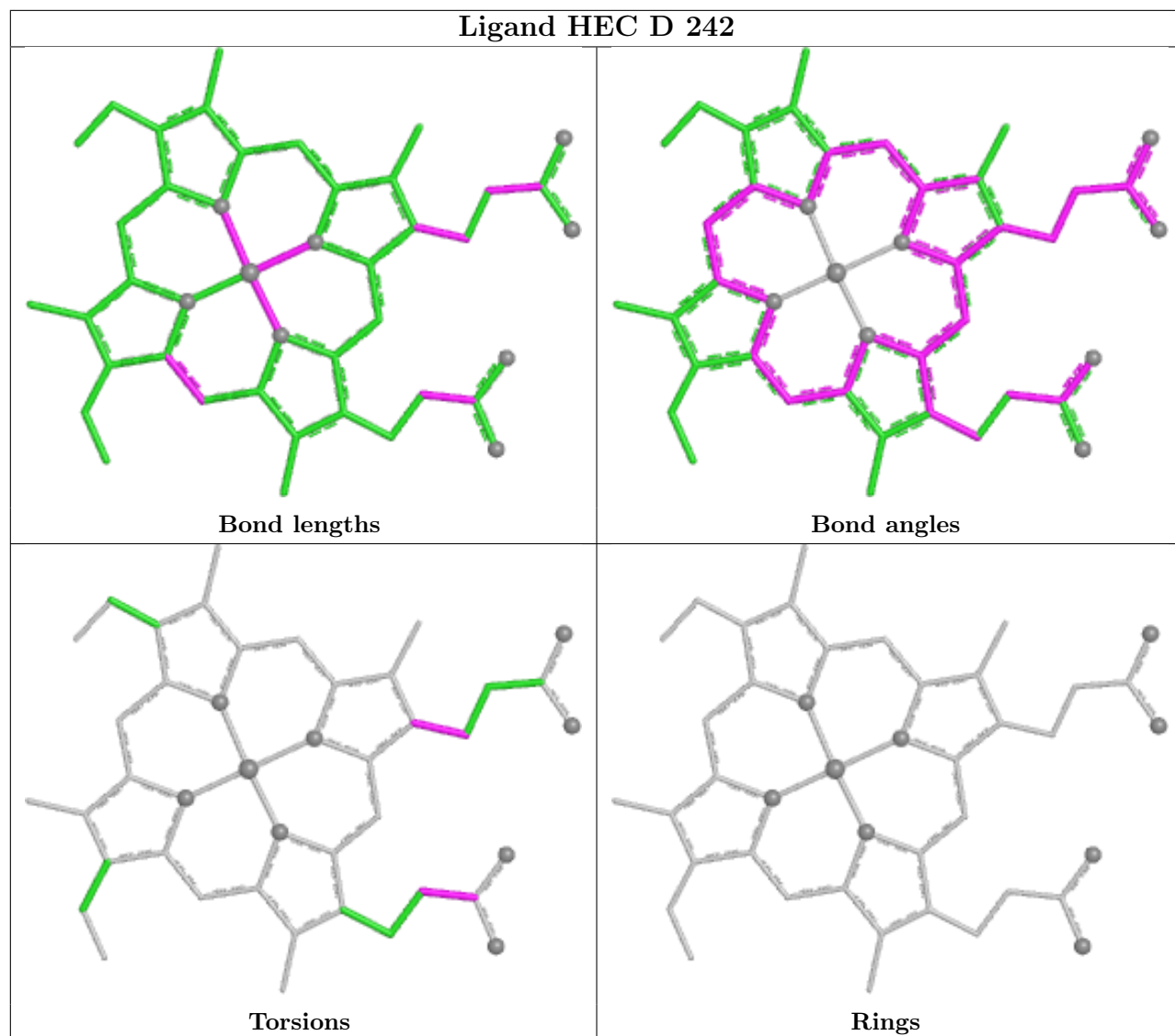
Bond angles



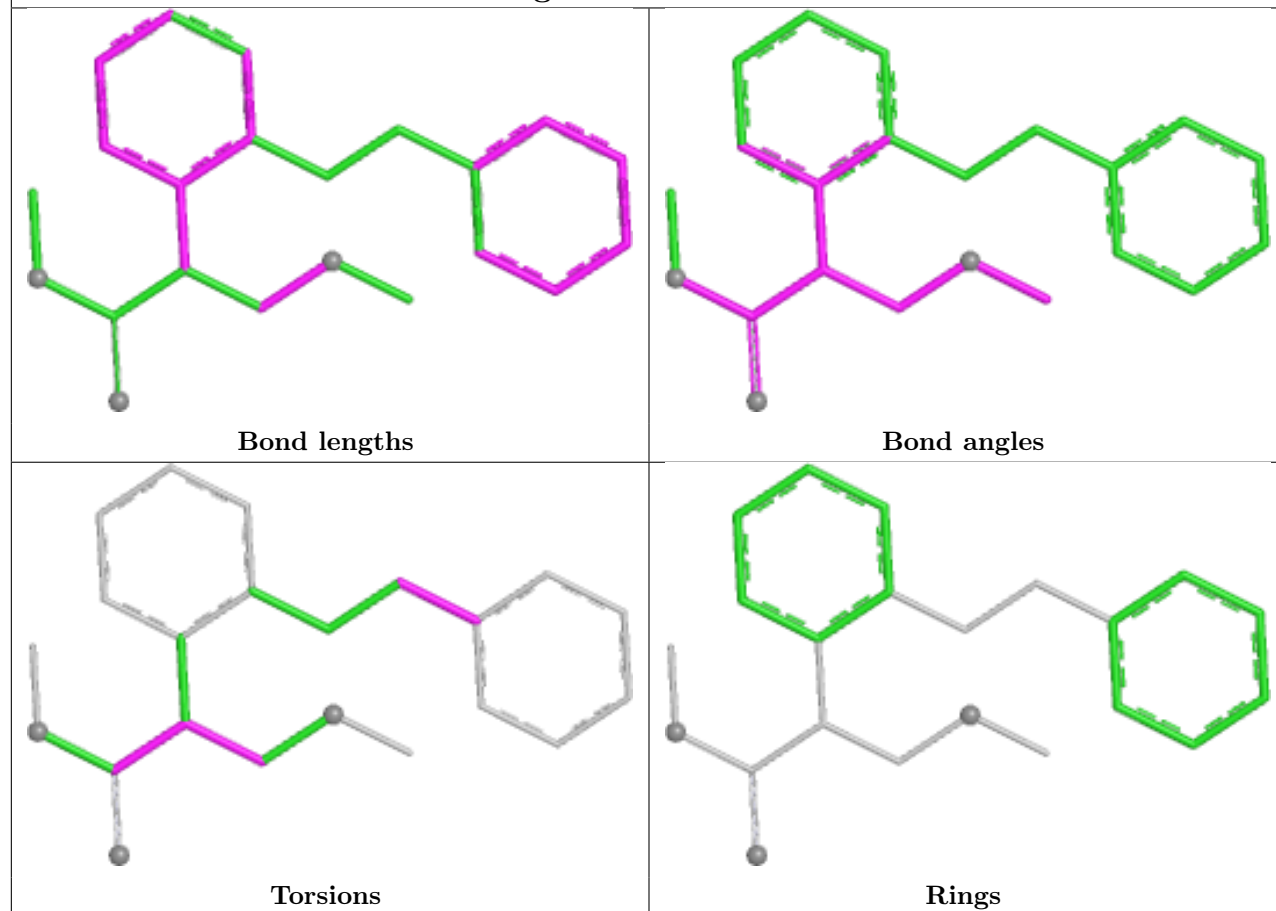
Torsions



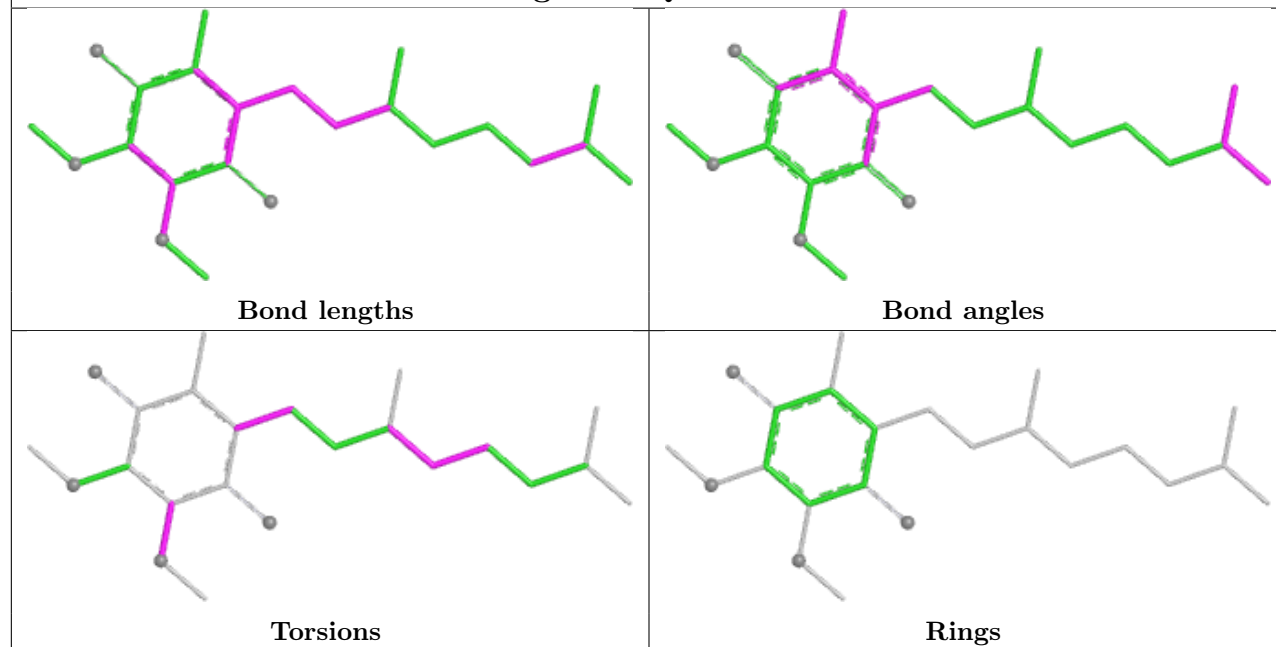
Rings



Ligand OST C 384



Ligand UQ2 C 383



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.