



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 01:17 PM EDT

PDB ID : 1SQV / pdb_00001sqv
Title : Crystal Structure Analysis of Bovine Bcl with UHDBT
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 : 2.85 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

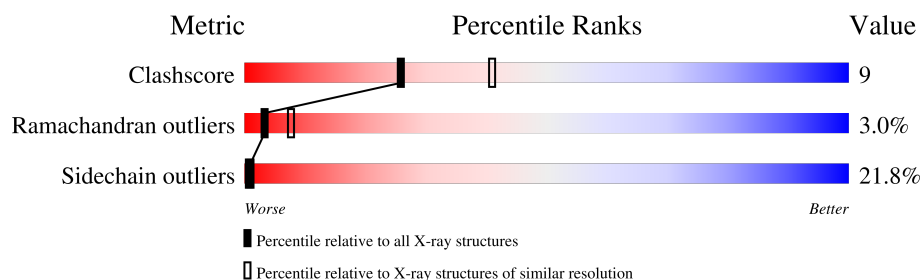
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)

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	
2	B	439	
3	C	379	
4	D	241	
5	E	196	
6	F	110	
7	G	81	
8	H	78	

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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	-	-	-
12	HEC	C	382	X	-	-	-
12	HEC	D	242	X	-	-	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 16953 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.

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.

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.

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	67	Total	C	N	O	S	0	0	0
			548	332	99	112	5			

- Molecule 9 is a protein called Ubiquinol-cytochrome C reductase complex 8 kDa protein.

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

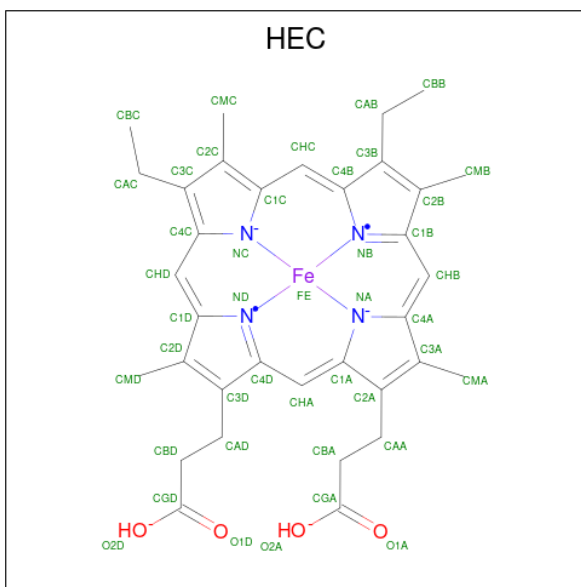
- Molecule 10 is a protein called Ubiquinol-cytochrome C reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	61	Total	C	N	O	S	0	0	0
			502	329	87	86				

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

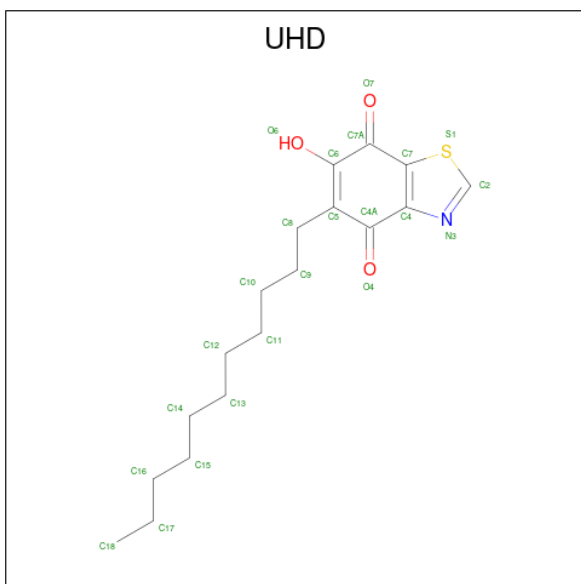
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	51	Total	C	N	O	S	0	0	0
			418	278	75	64	1			

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



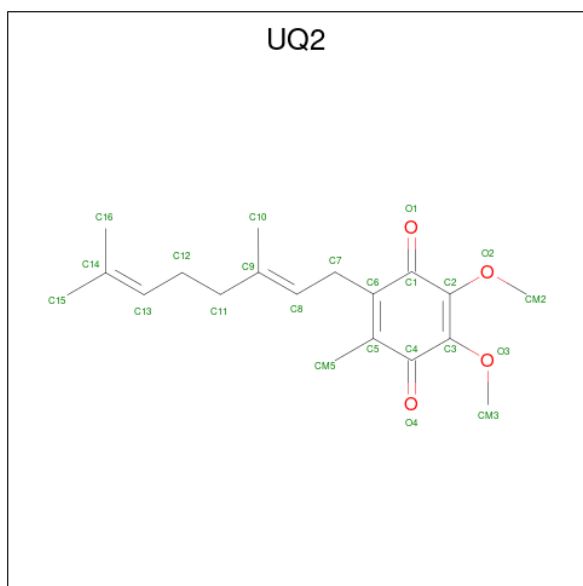
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 13 is 6-HYDROXY-5-UNDECYL-1,3-BENZOTHIAZOLE-4,7-DIONE (CCD ID: UHD) (formula: $C_{18}H_{25}NO_3S$).



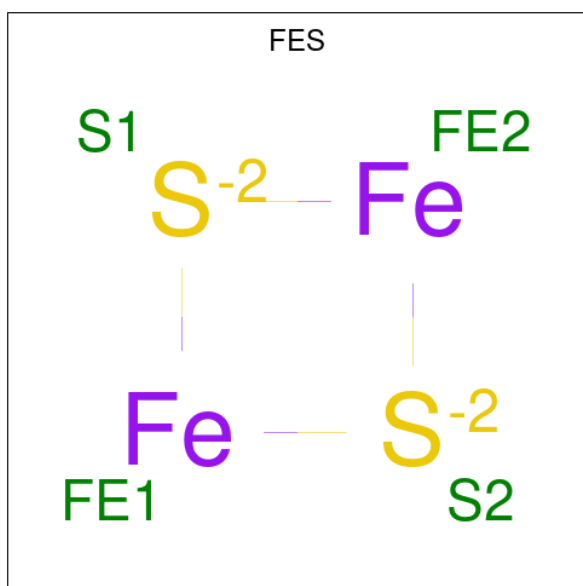
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	N	O	S	0	0
			23	18	1	3	1		

- Molecule 14 is UBIQUINONE-2 (CCD ID: UQ2) (formula: $C_{19}H_{26}O_4$).



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

- 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.

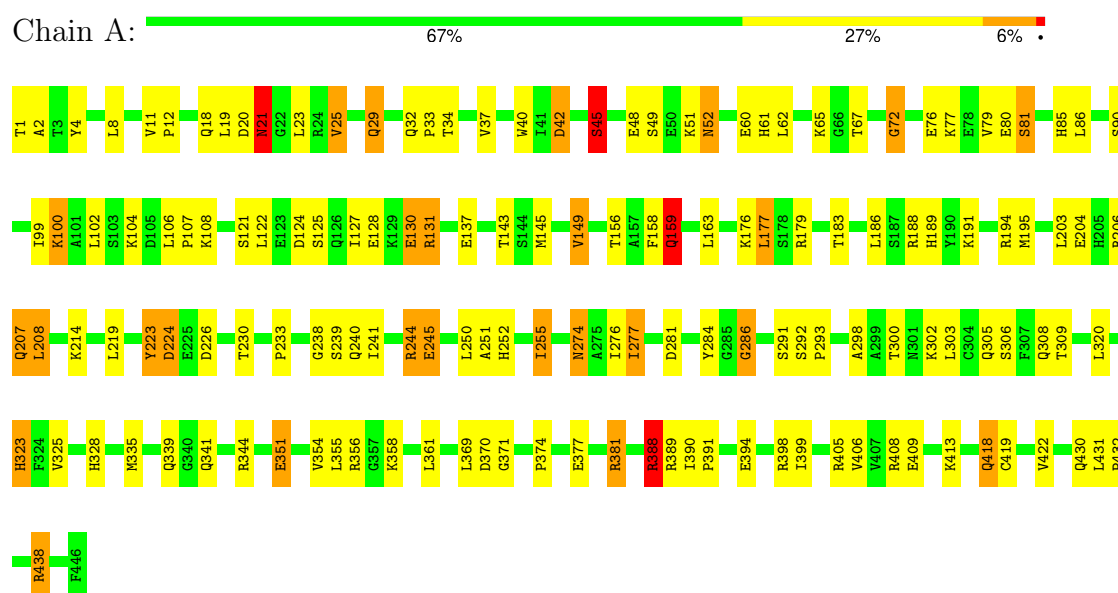
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	70	Total	O	0	0
			70	70		
16	B	103	Total	O	0	0
			103	103		
16	C	26	Total	O	0	0
			26	26		
16	D	21	Total	O	0	0
			21	21		
16	E	8	Total	O	0	0
			8	8		
16	F	31	Total	O	0	0
			31	31		
16	G	16	Total	O	0	0
			16	16		
16	I	10	Total	O	0	0
			10	10		
16	K	6	Total	O	0	0
			6	6		

3 Residue-property plots

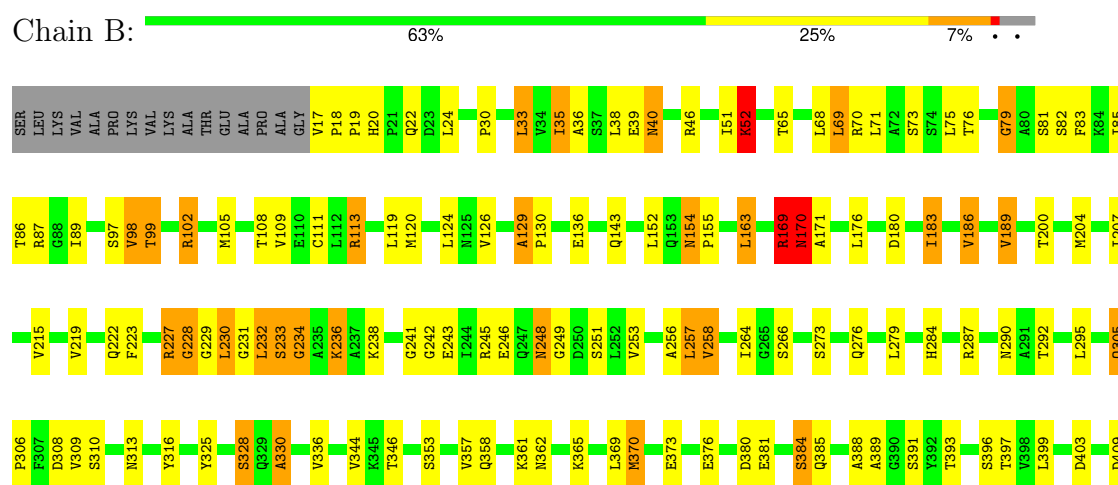
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



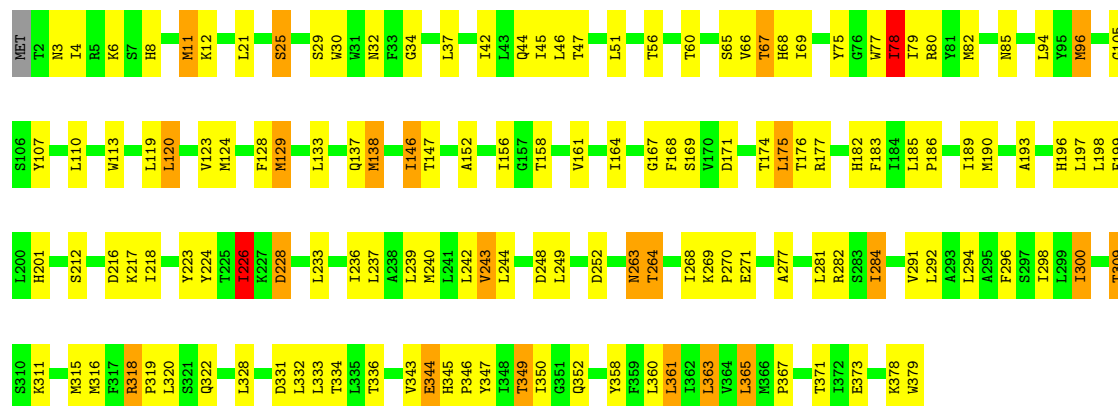
- Molecule 2: Ubiquinol-cytochrome c reductase complex core protein 2, mitochondrial





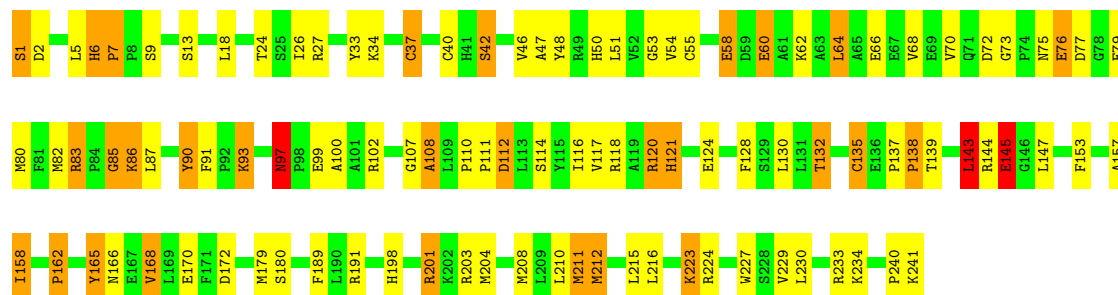
• Molecule 3: Cytochrome b

Chain C: 62% 31% 6% •



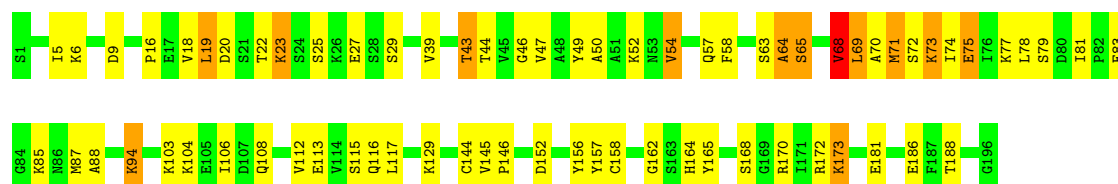
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D: 56% 30% 12% •



• Molecule 5: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain E: 64% 29% 6% •



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

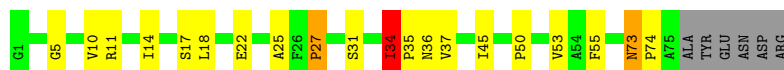
Chain F: 55% 32% 7% 5%





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

Chain G: 68% 21% 7%



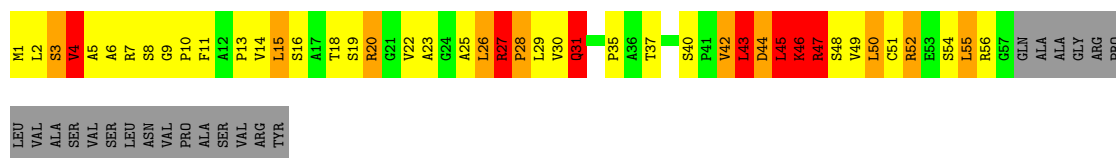
- Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein

Chain H: 55% 24% 6% 14%



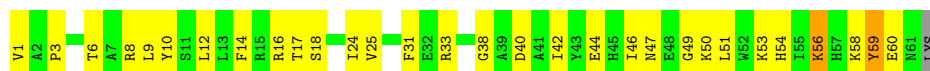
- Molecule 9: Ubiquinol-cytochrome C reductase complex 8 kDa protein

Chain I: 17% 35% 13% 9% 27%



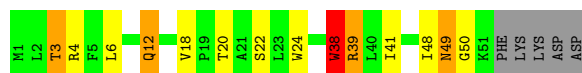
- Molecule 10: Ubiquinol-cytochrome C reductase complex 7.2 kDa protein

Chain J: 50% 45% 5%



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

Chain K: 66% 16% 7% 9%



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	153.67Å 153.67Å 589.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.85	Depositor
% Data completeness (in resolution range)	85.5 (40.00-2.85)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.217 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16953	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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: UHD, FES, HEC, UQ2

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	0.55	0/3531	1.16	3/4792 (0.1%)
2	B	0.66	0/3232	1.18	5/4386 (0.1%)
3	C	0.59	0/3100	1.27	6/4242 (0.1%)
4	D	0.59	0/1977	1.16	6/2684 (0.2%)
5	E	0.59	0/1553	1.14	2/2100 (0.1%)
6	F	0.60	0/930	1.19	1/1246 (0.1%)
7	G	0.87	1/649 (0.2%)	1.22	3/878 (0.3%)
8	H	0.57	0/553	1.20	1/741 (0.1%)
9	I	0.86	0/411	1.48	3/558 (0.5%)
10	J	0.59	0/515	1.18	0/696
11	K	0.61	0/433	1.23	0/594
All	All	0.62	1/16884 (0.0%)	1.20	30/22917 (0.1%)

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	8
2	B	0	12
3	C	0	3
4	D	0	21
5	E	0	5
6	F	0	1
8	H	0	5
9	I	0	16
10	J	0	1
11	K	0	3
All	All	0	75

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	34	ILE	CA-CB	15.62	1.61	1.54

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	34	ILE	N-CA-CB	9.79	117.08	110.52
4	D	7	PRO	N-CA-C	7.78	117.94	110.47
9	I	26	LEU	N-CA-C	7.48	121.25	109.81
7	G	50	PRO	N-CA-C	6.51	118.64	110.70
8	H	28	GLU	N-CA-C	6.16	118.78	111.33
3	C	226	ILE	N-CA-C	6.14	117.70	111.00
5	E	74	ILE	N-CA-C	6.08	117.05	108.17
4	D	162	PRO	N-CA-C	5.84	117.83	110.70
2	B	313	ASN	N-CA-C	5.83	118.69	107.44
3	C	345	HIS	N-CA-C	5.75	122.53	109.81
1	A	195	MET	N-CA-C	5.68	118.46	108.75
9	I	42	VAL	CB-CA-C	5.64	120.54	111.29
1	A	328	HIS	N-CA-C	5.51	118.81	111.75
3	C	78	ILE	N-CA-CB	5.46	116.93	110.55
4	D	201	ARG	N-CA-C	5.44	117.21	111.28
4	D	6	HIS	CA-C-N	5.36	123.57	119.66
4	D	6	HIS	C-N-CA	5.36	123.57	119.66
5	E	65	SER	N-CA-C	5.35	122.19	110.80
3	C	284	ILE	N-CA-C	5.23	113.69	107.73
3	C	199	PHE	N-CA-C	5.17	116.91	111.28
3	C	190	MET	N-CA-C	5.15	117.56	111.33
6	F	59	VAL	N-CA-CB	5.13	118.27	110.58
7	G	5	GLY	N-CA-C	-5.11	108.61	114.69
2	B	163	LEU	N-CA-C	-5.08	105.82	112.23
1	A	224	ASP	N-CA-C	5.07	121.60	110.80
2	B	330	ALA	N-CA-C	5.07	117.46	111.33
9	I	46	LYS	N-CA-C	5.05	117.38	108.75
2	B	189	VAL	N-CA-CB	5.04	117.39	110.54
2	B	79	GLY	N-CA-C	5.03	120.83	113.48
4	D	135	CYS	N-CA-C	5.01	114.91	108.34

There are no chirality outliers.

All (75) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	A	137	GLU	Mainchain
1	A	158	PHE	Peptide
1	A	20	ASP	Peptide
1	A	238	GLY	Peptide
1	A	388	ARG	Peptide
1	A	45	SER	Peptide
1	A	52	ASN	Peptide
2	B	108	THR	Mainchain
2	B	169	ARG	Peptide
2	B	19	PRO	Peptide
2	B	228	GLY	Peptide
2	B	231	GLY	Peptide
2	B	233	SER	Peptide
2	B	234	GLY	Peptide
2	B	248	ASN	Peptide
2	B	30	PRO	Mainchain
2	B	39	GLU	Peptide
2	B	436	ILE	Peptide
2	B	79	GLY	Peptide
3	C	167	GLY	Peptide
3	C	25	SER	Peptide
3	C	344	GLU	Peptide
4	D	1	SER	Peptide
4	D	107	GLY	Peptide
4	D	121	HIS	Peptide
4	D	137	PRO	Peptide
4	D	143	LEU	Peptide
4	D	144	ARG	Peptide
4	D	145	GLU	Peptide
4	D	157	ALA	Peptide
4	D	158	ILE	Peptide
4	D	162	PRO	Peptide
4	D	165	TYR	Peptide
4	D	168	VAL	Peptide
4	D	172	ASP	Peptide
4	D	240	PRO	Peptide
4	D	53	GLY	Peptide
4	D	73	GLY	Peptide
4	D	85	GLY	Peptide
4	D	86	LYS	Peptide
4	D	90	TYR	Peptide
4	D	93	LYS	Peptide

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Mol	Chain	Res	Type	Group
4	D	97	ASN	Peptide
5	E	63	SER	Peptide
5	E	64	ALA	Peptide
5	E	68	VAL	Peptide
5	E	70	ALA	Peptide
5	E	94	LYS	Peptide
6	F	6	VAL	Peptide
8	H	26	GLN	Peptide
8	H	27	LEU	Peptide
8	H	43	ARG	Peptide
8	H	48	SER	Peptide
8	H	52	GLU	Peptide
9	I	23	ALA	Peptide
9	I	25	ALA	Peptide
9	I	26	LEU	Peptide
9	I	28	PRO	Peptide
9	I	29	LEU	Peptide
9	I	3	SER	Peptide
9	I	31	GLN	Peptide
9	I	35	PRO	Peptide
9	I	37	THR	Peptide
9	I	4	VAL	Peptide
9	I	44	ASP	Peptide
9	I	45	LEU	Peptide
9	I	46	LYS	Peptide
9	I	52	ARG	Peptide
9	I	55	LEU	Peptide
9	I	6	ALA	Peptide
10	J	59	TYR	Peptide
11	K	3	THR	Peptide
11	K	38	TRP	Peptide
11	K	50	GLY	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	3356	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3172	0	3152	89	0
3	C	3003	0	3065	70	0
4	D	1918	0	1870	36	0
5	E	1519	0	1503	22	0
6	F	911	0	904	19	0
7	G	628	0	636	8	0
8	H	548	0	530	4	0
9	I	406	0	437	36	0
10	J	502	0	505	7	0
11	K	418	0	425	4	0
12	C	86	0	64	11	0
12	D	43	0	32	4	0
13	C	23	0	24	3	0
14	C	23	0	26	1	0
15	E	4	0	0	0	0
16	A	70	0	0	3	0
16	B	103	0	0	5	0
16	C	26	0	0	1	0
16	D	21	0	0	0	0
16	E	8	0	0	0	0
16	F	31	0	0	2	0
16	G	16	0	0	0	0
16	I	10	0	0	2	0
16	K	6	0	0	0	0
All	All	16953	0	16529	315	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 (315) 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)
4:D:211:MET:HE1	10:J:31:PHE:HE2	1.33	0.93
16:B:623:HOH:O	9:I:11:PHE:HB2	1.70	0.92
2:B:310:SER:HB3	9:I:28:PRO:HD3	1.52	0.90
16:B:627:HOH:O	9:I:4:VAL:HG21	1.75	0.85
2:B:385:GLN:HA	9:I:2:LEU:HD12	1.60	0.81
2:B:388:ALA:HB3	9:I:2:LEU:HD13	1.64	0.80
2:B:76:THR:HG22	2:B:82:SER:H	1.46	0.80
2:B:215:VAL:O	2:B:219:VAL:HG23	1.84	0.77
4:D:211:MET:HE1	10:J:31:PHE:CE2	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:THR:HB	9:I:14:VAL:HG22	1.69	0.74
3:C:309:THR:HG21	3:C:367:PRO:O	1.88	0.73
5:E:156:TYR:HB2	5:E:165:TYR:HB2	1.70	0.73
2:B:46:ARG:HG3	2:B:46:ARG:HH11	1.54	0.72
5:E:20:ASP:HB3	5:E:23:LYS:HB2	1.72	0.72
2:B:264:ILE:HD11	9:I:2:LEU:HA	1.71	0.71
1:A:145:MET:O	1:A:149:VAL:HG23	1.90	0.70
2:B:170:ASN:HD22	2:B:238:LYS:H	1.38	0.69
2:B:169:ARG:HD2	2:B:238:LYS:HE2	1.74	0.68
1:A:61:HIS:HB3	1:A:130:GLU:HG3	1.76	0.68
1:A:255:ILE:HD13	1:A:335:MET:HE1	1.76	0.67
6:F:96:GLU:O	6:F:100:GLU:HG3	1.94	0.67
6:F:38:HIS:HB3	16:F:750:HOH:O	1.95	0.66
3:C:75:TYR:HB3	3:C:78:ILE:HD11	1.78	0.65
1:A:156:THR:O	1:A:159:GLN:HB2	1.96	0.65
1:A:240:GLN:HG3	1:A:422:VAL:HB	1.79	0.64
1:A:244:ARG:NH2	16:A:514:HOH:O	2.10	0.64
3:C:30:TRP:HZ3	3:C:96:MET:HG3	1.63	0.64
16:A:530:HOH:O	9:I:42:VAL:HG12	1.97	0.63
1:A:308:GLN:HE21	1:A:323:HIS:CD2	2.17	0.63
1:A:308:GLN:HE21	1:A:323:HIS:HD2	1.45	0.62
2:B:385:GLN:NE2	2:B:393:THR:H	1.97	0.62
2:B:126:VAL:O	2:B:130:PRO:HG3	1.99	0.62
7:G:73:ASN:HB3	7:G:74:PRO:HD3	1.82	0.62
1:A:149:VAL:HG21	1:A:252:HIS:HB3	1.82	0.62
6:F:65:ALA:HA	6:F:68:LEU:HD12	1.81	0.61
2:B:176:LEU:HD13	9:I:13:PRO:CD	2.31	0.61
1:A:281:ASP:OD1	9:I:47:ARG:HA	2.01	0.61
2:B:76:THR:CG2	2:B:82:SER:H	2.14	0.61
3:C:237:LEU:HD13	4:D:212:MET:HG2	1.83	0.60
2:B:385:GLN:HE22	2:B:393:THR:H	1.49	0.60
1:A:29:GLN:HG2	2:B:18:PRO:HD3	1.83	0.60
3:C:47:THR:HG22	5:E:58:PHE:HZ	1.67	0.60
3:C:233:LEU:CD2	4:D:216:LEU:HG	2.31	0.60
2:B:258:VAL:HG12	2:B:423:SER:HB2	1.84	0.59
3:C:77:TRP:CZ3	4:D:201:ARG:HB3	2.37	0.59
2:B:245:ARG:NH2	2:B:433:THR:O	2.35	0.59
4:D:70:VAL:HB	4:D:83:ARG:HB3	1.85	0.59
10:J:10:TYR:HA	10:J:14:PHE:HB2	1.83	0.59
3:C:25:SER:HA	3:C:218:ILE:HG12	1.85	0.58
1:A:244:ARG:NE	16:A:514:HOH:O	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:20:ARG:HG3	9:I:51:CYS:SG	2.42	0.58
8:H:62:LEU:HD23	8:H:65:ARG:HH12	1.67	0.58
2:B:264:ILE:HG12	9:I:2:LEU:HD22	1.85	0.58
3:C:224:TYR:O	3:C:228:ASP:HB2	2.03	0.58
1:A:335:MET:HE3	1:A:339:GLN:HG3	1.85	0.58
3:C:3:ASN:HB3	3:C:6:LYS:HG3	1.85	0.58
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.44	0.58
3:C:119:LEU:HB3	12:C:382:HEC:HBB3	1.85	0.57
2:B:40:ASN:C	2:B:40:ASN:HD22	2.12	0.57
2:B:76:THR:HG22	2:B:82:SER:N	2.18	0.57
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.86	0.57
4:D:60:GLU:O	4:D:64:LEU:HG	2.05	0.56
2:B:129:ALA:N	2:B:130:PRO:HD3	2.21	0.56
1:A:351:GLU:H	11:K:12:GLN:HE21	1.54	0.56
11:K:38:TRP:HD1	11:K:41:ILE:CD1	2.19	0.55
9:I:28:PRO:HA	9:I:30:VAL:HG22	1.88	0.55
1:A:45:SER:HA	1:A:48:GLU:HG2	1.88	0.55
3:C:361:LEU:HA	3:C:365:LEU:HB2	1.89	0.55
1:A:371:GLY:O	1:A:374:PRO:HD2	2.08	0.54
2:B:76:THR:HG22	2:B:81:SER:HA	1.89	0.54
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.43	0.54
5:E:168:SER:HB3	5:E:170:ARG:HG3	1.88	0.54
2:B:69:LEU:CD1	2:B:105:MET:HE1	2.38	0.54
11:K:38:TRP:HA	11:K:38:TRP:CE3	2.41	0.53
3:C:216:ASP:OD2	4:D:233:ARG:NH2	2.40	0.53
1:A:419:CYS:SG	1:A:438:ARG:NH1	2.81	0.53
2:B:111:CYS:SG	2:B:119:LEU:HD12	2.49	0.53
3:C:34:GLY:HA3	12:C:382:HEC:HBA2	1.91	0.53
1:A:281:ASP:HB3	1:A:284:TYR:CD1	2.44	0.53
1:A:2:ALA:O	2:B:113:ARG:HD3	2.08	0.53
3:C:45:ILE:HA	12:C:381:HEC:HAB	1.90	0.52
3:C:137:GLN:HE22	3:C:263:ASN:HB3	1.75	0.52
2:B:111:CYS:HB3	2:B:119:LEU:HD12	1.91	0.52
3:C:296:PHE:O	3:C:300:ILE:HB	2.09	0.52
2:B:52:LYS:HD3	2:B:233:SER:OG	2.09	0.52
6:F:106:GLU:HA	6:F:109:LYS:HD2	1.91	0.52
3:C:147:THR:HG22	3:C:161:VAL:HG13	1.92	0.52
2:B:69:LEU:HD13	2:B:105:MET:HE1	1.92	0.52
2:B:279:LEU:HB3	2:B:295:LEU:HG	1.92	0.52
2:B:328:SER:HB3	2:B:336:VAL:HG21	1.92	0.52
3:C:29:SER:HA	3:C:32:ASN:HD22	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:382:HEC:HMC1	12:C:382:HEC:HBC3	1.92	0.52
4:D:97:ASN:HB3	4:D:100:ALA:H	1.75	0.52
3:C:186:PRO:HG2	12:C:381:HEC:HBB2	1.92	0.52
3:C:77:TRP:CH2	4:D:204:MET:HE2	2.45	0.51
9:I:43:LEU:HA	9:I:46:LYS:HD3	1.91	0.51
1:A:25:VAL:HG23	1:A:208:LEU:HD13	1.91	0.51
1:A:49:SER:H	1:A:52:ASN:HB2	1.75	0.51
4:D:108:ALA:HB1	12:D:242:HEC:HMD3	1.91	0.51
1:A:65:LYS:O	1:A:72:GLY:HA2	2.11	0.51
1:A:80:GLU:HG2	2:B:284:HIS:HB2	1.93	0.51
3:C:300:ILE:HD11	3:C:363:LEU:HD13	1.92	0.51
3:C:113:TRP:HA	12:C:382:HEC:HHD	1.93	0.51
5:E:50:ALA:O	5:E:54:VAL:HG23	2.11	0.51
2:B:246:GLU:O	2:B:427:SER:HA	2.11	0.50
4:D:99:GLU:HA	4:D:102:ARG:HB2	1.94	0.50
1:A:21:ASN:HB3	1:A:23:LEU:H	1.76	0.50
6:F:51:PRO:HD2	6:F:54:LEU:HD12	1.94	0.50
2:B:85:ILE:O	2:B:89:ILE:HG13	2.12	0.50
4:D:42:SER:HB2	4:D:112:ASP:HB3	1.94	0.50
5:E:18:VAL:HG11	7:G:22:GLU:OE1	2.10	0.50
2:B:170:ASN:ND2	2:B:238:LYS:H	2.07	0.50
2:B:176:LEU:HD13	9:I:13:PRO:HD3	1.93	0.50
6:F:67:ASP:O	6:F:71:ARG:HG2	2.12	0.50
4:D:47:ALA:N	4:D:50:HIS:HD2	2.09	0.50
4:D:128:PHE:O	4:D:132:THR:HB	2.12	0.50
6:F:82:LYS:HB2	6:F:85:GLU:HB2	1.93	0.50
1:A:48:GLU:HB2	1:A:52:ASN:HB3	1.94	0.49
1:A:291:SER:HB3	1:A:356:ARG:CZ	2.42	0.49
2:B:68:LEU:HD23	2:B:186:VAL:HG22	1.94	0.49
1:A:19:LEU:HB3	1:A:21:ASN:HB2	1.93	0.49
1:A:240:GLN:HB3	7:G:17:SER:HB2	1.93	0.49
3:C:138:MET:HE1	3:C:271:GLU:HG2	1.94	0.49
1:A:255:ILE:HD13	1:A:335:MET:CE	2.41	0.49
2:B:33:LEU:HD23	2:B:35:ILE:HD11	1.95	0.49
2:B:102:ARG:HD2	16:B:641:HOH:O	2.11	0.49
5:E:69:LEU:HD12	5:E:71:MET:HE2	1.93	0.49
1:A:277:ILE:HB	1:A:309:THR:HG21	1.94	0.49
1:A:281:ASP:HB3	1:A:284:TYR:CE1	2.48	0.49
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.94	0.49
3:C:319:PRO:HA	3:C:322:GLN:HB2	1.95	0.49
2:B:169:ARG:HG3	2:B:238:LYS:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:197:LEU:HD21	14:C:384:UQ2:H5M2	1.94	0.49
6:F:28:LYS:HB3	6:F:74:ILE:HG13	1.94	0.49
1:A:418:GLN:HE21	1:A:418:GLN:HA	1.78	0.49
2:B:242:GLY:O	2:B:423:SER:HA	2.12	0.49
2:B:424:MET:HB2	2:B:436:ILE:HD11	1.95	0.48
4:D:215:LEU:HD21	5:E:46:GLY:HA3	1.95	0.48
5:E:157:TYR:CE1	5:E:162:GLY:HA2	2.47	0.48
3:C:44:GLN:HG3	12:C:381:HEC:HBC2	1.94	0.48
3:C:349:THR:HA	3:C:352:GLN:HE21	1.78	0.48
10:J:33:ARG:HD3	11:K:48:ILE:HA	1.95	0.48
1:A:189:HIS:O	1:A:194:ARG:NH1	2.46	0.48
1:A:284:TYR:HE1	9:I:20:ARG:HG2	1.78	0.48
2:B:89:ILE:HG12	2:B:119:LEU:HD21	1.95	0.48
5:E:164:HIS:HB2	5:E:173:LYS:HB2	1.95	0.48
1:A:79:VAL:HG11	1:A:86:LEU:HB2	1.94	0.48
3:C:128:PHE:CD1	3:C:146:ILE:HD12	2.48	0.48
3:C:270:PRO:HB3	13:C:383:UHD:O4	2.13	0.48
2:B:97:SER:HB2	9:I:15:LEU:O	2.14	0.48
2:B:369:LEU:HD11	2:B:399:LEU:HD11	1.96	0.48
12:C:382:HEC:HMC1	12:C:382:HEC:CBC	2.44	0.48
4:D:138:PRO:HB3	8:H:58:LEU:HD13	1.96	0.48
12:D:242:HEC:HMB3	12:D:242:HEC:HBB3	1.96	0.48
1:A:341:GLN:HE22	1:A:344:ARG:HH21	1.62	0.48
2:B:70:ARG:HG3	2:B:98:VAL:HG22	1.95	0.48
4:D:26:ILE:HG23	4:D:189:PHE:HA	1.95	0.48
12:D:242:HEC:HMB3	12:D:242:HEC:CBB	2.43	0.47
6:F:28:LYS:HB3	6:F:74:ILE:CG1	2.43	0.47
1:A:431:LEU:HD12	1:A:432:PRO:HD2	1.96	0.47
2:B:385:GLN:NE2	2:B:393:THR:N	2.62	0.47
4:D:48:TYR:HA	4:D:51:LEU:HD12	1.96	0.47
7:G:34:ILE:HG13	7:G:35:PRO:HD3	1.95	0.47
1:A:77:LYS:O	1:A:81:SER:HB2	2.15	0.47
1:A:252:HIS:CE1	9:I:43:LEU:HB2	2.49	0.47
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.95	0.47
1:A:149:VAL:HG21	1:A:252:HIS:CB	2.42	0.47
2:B:365:LYS:NZ	2:B:403:ASP:OD1	2.30	0.47
2:B:389:ALA:HB2	9:I:2:LEU:HD11	1.96	0.47
3:C:186:PRO:HA	3:C:189:ILE:HD12	1.97	0.47
9:I:1:MET:SD	16:I:671:HOH:O	2.60	0.47
2:B:99:THR:HB	9:I:14:VAL:CG2	2.43	0.47
2:B:253:VAL:HG23	2:B:330:ALA:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:124:GLU:CD	4:D:191:ARG:HD3	2.39	0.47
1:A:131:ARG:NH2	1:A:177:LEU:O	2.44	0.46
9:I:16:SER:HB3	9:I:19:SER:O	2.15	0.46
3:C:65:SER:O	3:C:68:HIS:HB3	2.16	0.46
2:B:305:GLN:HB2	2:B:306:PRO:HD2	1.97	0.46
3:C:8:HIS:HD2	3:C:11:MET:H	1.62	0.46
3:C:315:MET:HA	3:C:318:ARG:HG3	1.98	0.46
3:C:244:LEU:HD22	4:D:204:MET:HB2	1.98	0.46
6:F:35:ASP:OD2	6:F:61:ARG:HD2	2.16	0.46
1:A:62:LEU:HD13	1:A:122:LEU:HD23	1.96	0.46
1:A:122:LEU:HB2	1:A:179:ARG:HE	1.81	0.46
2:B:36:ALA:O	2:B:207:ILE:HA	2.15	0.46
5:E:87:MET:HE3	5:E:88:ALA:H	1.81	0.46
3:C:67:THR:HG23	16:C:685:HOH:O	2.15	0.46
1:A:388:ARG:NH2	1:A:394:GLU:OE1	2.49	0.45
4:D:33:TYR:HA	4:D:37:CYS:SG	2.55	0.45
3:C:119:LEU:HD13	12:C:382:HEC:HBB3	1.98	0.45
4:D:110:PRO:HA	4:D:111:PRO:HD3	1.82	0.45
2:B:180:ASP:HA	2:B:183:ILE:HG13	1.97	0.45
1:A:85:HIS:HB2	1:A:100:LYS:HB2	1.97	0.45
9:I:43:LEU:HD23	9:I:46:LYS:HZ3	1.82	0.45
3:C:146:ILE:HG12	13:C:383:UHD:H82	1.97	0.45
1:A:388:ARG:HH22	1:A:394:GLU:CD	2.24	0.45
4:D:75:ASN:O	4:D:77:ASP:N	2.48	0.45
9:I:11:PHE:HZ	9:I:27:ARG:CZ	2.30	0.45
2:B:435:PHE:O	2:B:436:ILE:HB	2.17	0.45
1:A:355:LEU:HA	1:A:358:LYS:HE3	1.99	0.45
2:B:325:TYR:HB3	9:I:28:PRO:HD2	1.98	0.45
2:B:316:TYR:OH	9:I:10:PRO:HB3	2.17	0.44
3:C:373:GLU:HB3	6:F:20:TYR:OH	2.18	0.44
9:I:4:VAL:HG12	9:I:10:PRO:HG3	1.99	0.44
3:C:332:LEU:HD21	3:C:358:TYR:CE1	2.52	0.44
4:D:108:ALA:HB1	12:D:242:HEC:HAD1	2.00	0.44
1:A:361:LEU:HD23	1:A:399:ILE:HG12	1.98	0.44
3:C:47:THR:HG22	5:E:58:PHE:CZ	2.50	0.44
2:B:65:THR:O	2:B:69:LEU:HB2	2.18	0.44
2:B:120:MET:HE3	2:B:219:VAL:HG21	2.00	0.44
8:H:65:ARG:HB3	8:H:65:ARG:HH11	1.83	0.44
1:A:11:VAL:HA	1:A:12:PRO:HD3	1.86	0.44
2:B:380:ASP:O	2:B:384:SER:OG	2.36	0.44
7:G:25:ALA:O	7:G:27:PRO:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:ASN:HA	2:B:155:PRO:HD2	1.85	0.44
2:B:176:LEU:HD13	9:I:13:PRO:HD2	1.98	0.44
3:C:51:LEU:HD13	12:C:381:HEC:HBA1	2.00	0.44
3:C:270:PRO:HB3	13:C:383:UHD:C4A	2.48	0.44
6:F:68:LEU:HD21	6:F:75:LEU:HD23	2.00	0.44
9:I:51:CYS:SG	9:I:52:ARG:N	2.91	0.44
2:B:33:LEU:HD23	2:B:35:ILE:CD1	2.48	0.43
3:C:75:TYR:HB3	3:C:78:ILE:CD1	2.47	0.43
3:C:331:ASP:O	3:C:334:THR:HB	2.17	0.43
3:C:240:MET:HB3	4:D:208:MET:HG3	2.00	0.43
3:C:119:LEU:O	3:C:123:VAL:HG12	2.18	0.43
2:B:143:GLN:O	2:B:143:GLN:HG3	2.19	0.43
2:B:256:ALA:HB2	2:B:325:TYR:CD2	2.54	0.43
5:E:145:VAL:HA	5:E:146:PRO:HD3	1.86	0.43
2:B:264:ILE:HG22	2:B:316:TYR:C	2.44	0.43
3:C:82:MET:HG2	3:C:240:MET:HE1	2.00	0.43
3:C:85:ASN:HD22	3:C:243:VAL:HG12	1.84	0.43
3:C:233:LEU:HD22	4:D:216:LEU:HG	1.99	0.43
4:D:117:VAL:HG11	4:D:191:ARG:HD2	2.01	0.43
6:F:90:LEU:O	6:F:91:GLU:C	2.62	0.43
1:A:286:GLY:HA3	16:B:659:HOH:O	2.18	0.43
2:B:99:THR:CB	9:I:14:VAL:HG22	2.44	0.43
2:B:241:GLY:HA2	2:B:423:SER:OG	2.18	0.43
3:C:233:LEU:HA	3:C:236:ILE:HD12	2.00	0.43
2:B:119:LEU:HA	2:B:119:LEU:HD23	1.60	0.43
3:C:129:MET:HB3	3:C:182:HIS:HB2	2.00	0.43
6:F:72:GLN:HE21	6:F:72:GLN:HA	1.84	0.43
2:B:257:LEU:HD23	2:B:424:MET:HG3	2.00	0.43
3:C:223:TYR:CE1	4:D:230:LEU:HD12	2.54	0.43
5:E:75:GLU:H	5:E:75:GLU:HG2	1.65	0.42
2:B:325:TYR:CD1	9:I:28:PRO:HD2	2.54	0.42
2:B:370:MET:O	2:B:373:GLU:HB2	2.19	0.42
6:F:33:ARG:O	6:F:36:THR:OG1	2.35	0.42
3:C:105:GLY:HA2	3:C:107:TYR:CE2	2.55	0.42
2:B:124:LEU:HD11	2:B:219:VAL:CG1	2.50	0.42
9:I:1:MET:HB3	16:I:671:HOH:O	2.20	0.42
1:A:292:SER:HA	1:A:293:PRO:HD3	1.84	0.42
1:A:430:GLN:O	1:A:430:GLN:HG2	2.20	0.42
2:B:73:SER:HB3	2:B:98:VAL:HG11	2.01	0.42
3:C:75:TYR:CE1	5:E:57:GLN:HG2	2.55	0.42
3:C:193:ALA:O	3:C:196:HIS:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:120:ARG:HA	4:D:120:ARG:HD3	1.79	0.42
1:A:233:PRO:HB2	5:E:22:THR:O	2.19	0.42
1:A:281:ASP:HB2	9:I:20:ARG:NE	2.35	0.42
1:A:390:ILE:HA	1:A:391:PRO:HD3	1.87	0.42
2:B:381:GLU:OE1	2:B:381:GLU:HA	2.20	0.42
4:D:211:MET:HE3	5:E:49:TYR:CD1	2.55	0.42
2:B:200:THR:HG21	2:B:229:GLY:H	1.85	0.42
3:C:311:LYS:HE3	6:F:37:ILE:HD11	2.02	0.42
2:B:83:PHE:CZ	2:B:87:ARG:HG3	2.55	0.42
3:C:197:LEU:HD22	3:C:201:HIS:CE1	2.54	0.42
10:J:47:ASN:HB3	10:J:50:LYS:HB2	2.00	0.42
1:A:79:VAL:HG21	1:A:86:LEU:HD22	2.02	0.42
6:F:47:ILE:H	6:F:47:ILE:HG12	1.58	0.42
6:F:64:ARG:HB3	16:F:749:HOH:O	2.20	0.42
1:A:156:THR:HG21	1:A:241:ILE:HG22	2.02	0.41
2:B:243:GLU:HA	2:B:424:MET:O	2.20	0.41
3:C:37:LEU:HD22	12:C:382:HEC:HAB	2.02	0.41
5:E:39:VAL:O	5:E:43:THR:OG1	2.38	0.41
1:A:245:GLU:CD	7:G:11:ARG:HH21	2.26	0.41
1:A:381:ARG:HH22	9:I:56:ARG:HD2	1.86	0.41
2:B:227:ARG:NH2	2:B:230:LEU:O	2.45	0.41
2:B:365:LYS:HG2	2:B:399:LEU:HD22	2.01	0.41
3:C:277:ALA:HB1	3:C:294:LEU:HD11	2.02	0.41
1:A:4:TYR:CZ	1:A:8:LEU:HD11	2.54	0.41
1:A:67:THR:HA	1:A:121:SER:H	1.85	0.41
4:D:223:LYS:HD2	4:D:227:TRP:CD1	2.55	0.41
1:A:42:ASP:O	1:A:194:ARG:NH2	2.53	0.41
1:A:274:ASN:HD22	1:A:274:ASN:HA	1.54	0.41
3:C:226:ILE:HG23	4:D:223:LYS:HB2	2.02	0.41
10:J:38:GLY:O	10:J:42:ILE:HG12	2.21	0.41
3:C:66:VAL:HA	3:C:69:ILE:HD12	2.03	0.41
3:C:133:LEU:HA	3:C:175:LEU:HD21	2.01	0.41
1:A:207:GLN:H	1:A:207:GLN:HG3	1.73	0.41
2:B:305:GLN:CB	2:B:306:PRO:HD2	2.50	0.41
1:A:251:ALA:O	1:A:325:VAL:HA	2.21	0.41
1:A:255:ILE:HD12	1:A:422:VAL:HG22	2.02	0.41
2:B:222:GLN:HB3	2:B:223:PHE:CD2	2.56	0.41
3:C:152:ALA:CB	3:C:291:VAL:HG11	2.50	0.41
4:D:143:LEU:HB2	4:D:145:GLU:H	1.85	0.41
6:F:59:VAL:HG21	7:G:10:VAL:HG13	2.03	0.41
1:A:341:GLN:NE2	1:A:344:ARG:HH21	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:308:ASP:OD1	9:I:31:GLN:HB2	2.20	0.41
3:C:8:HIS:CD2	3:C:11:MET:H	2.39	0.41
3:C:239:LEU:HG	3:C:240:MET:HE2	2.02	0.41
5:E:16:PRO:HA	5:E:19:LEU:HD12	2.02	0.41
1:A:60:GLU:OE2	2:B:287:ARG:NH2	2.54	0.41
2:B:126:VAL:HG22	16:B:626:HOH:O	2.21	0.41
2:B:200:THR:HB	2:B:227:ARG:HA	2.03	0.41
4:D:6:HIS:HA	4:D:7:PRO:HD3	1.96	0.41
4:D:83:ARG:HD2	4:D:85:GLY:H	1.85	0.41
3:C:94:LEU:HD22	3:C:120:LEU:HD12	2.03	0.40
3:C:183:PHE:O	3:C:186:PRO:HD2	2.21	0.40
3:C:334:THR:OG1	7:G:55:PHE:HD1	2.04	0.40
10:J:51:LEU:HB2	10:J:54:HIS:CE1	2.57	0.40
2:B:71:LEU:CD2	9:I:15:LEU:HG	2.51	0.40
5:E:43:THR:O	5:E:47:VAL:HG23	2.21	0.40
5:E:103:LYS:HA	5:E:106:ILE:HD12	2.02	0.40
8:H:66:ASP:HA	8:H:69:VAL:HB	2.03	0.40
3:C:105:GLY:HA2	3:C:107:TYR:CZ	2.56	0.40
1:A:276:ILE:HD11	1:A:354:VAL:HA	2.02	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%)	397 (89%)	37 (8%)	10 (2%)	5	11
2	B	421/439 (96%)	383 (91%)	26 (6%)	12 (3%)	3	8
3	C	376/379 (99%)	332 (88%)	39 (10%)	5 (1%)	9	21
4	D	239/241 (99%)	199 (83%)	30 (13%)	10 (4%)	2	3
5	E	194/196 (99%)	168 (87%)	21 (11%)	5 (3%)	4	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	103/110 (94%)	98 (95%)	3 (3%)	2 (2%)	6	14
7	G	73/81 (90%)	66 (90%)	5 (7%)	2 (3%)	4	9
8	H	65/78 (83%)	57 (88%)	7 (11%)	1 (2%)	8	18
9	I	55/78 (70%)	28 (51%)	17 (31%)	10 (18%)	0	0
10	J	59/62 (95%)	48 (81%)	8 (14%)	3 (5%)	1	2
11	K	49/56 (88%)	42 (86%)	4 (8%)	3 (6%)	1	2
All	All	2078/2166 (96%)	1818 (88%)	197 (10%)	63 (3%)	3	8

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
2	B	52	LYS
2	B	232	LEU
2	B	437	ASP
3	C	347	TYR
4	D	76	GLU
4	D	93	LYS
4	D	108	ALA
5	E	65	SER
8	H	26	GLN
9	I	4	VAL
9	I	5	ALA
9	I	27	ARG
9	I	45	LEU
9	I	47	ARG
11	K	4	ARG
11	K	39	ARG
1	A	21	ASN
1	A	72	GLY
1	A	125	SER
1	A	239	SER
1	A	286	GLY
2	B	249	GLY
4	D	58	GLU
4	D	87	LEU
4	D	90	TYR
5	E	68	VAL
9	I	43	LEU
10	J	56	LYS

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Mol	Chain	Res	Type
1	A	224	ASP
3	C	177	ARG
4	D	80	MET
4	D	138	PRO
7	G	73	ASN
10	J	3	PRO
1	A	223	TYR
2	B	171	ALA
2	B	236	LYS
2	B	436	ILE
3	C	12	LYS
4	D	198	HIS
5	E	73	LYS
6	F	27	ASN
7	G	27	PRO
10	J	49	GLY
1	A	107	PRO
5	E	64	ALA
5	E	83	GLU
6	F	91	GLU
9	I	31	GLN
1	A	33	PRO
2	B	170	ASN
2	B	266	SER
9	I	9	GLY
9	I	50	LEU
11	K	49	ASN
2	B	228	GLY
9	I	40	SER
2	B	129	ALA
3	C	264	THR
3	C	346	PRO
2	B	234	GLY
4	D	229	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/370 (100%)	300 (81%)	70 (19%)	1	2
2	B	332/343 (97%)	275 (83%)	57 (17%)	2	3
3	C	326/327 (100%)	260 (80%)	66 (20%)	1	2
4	D	206/206 (100%)	148 (72%)	58 (28%)	0	0
5	E	168/168 (100%)	130 (77%)	38 (23%)	1	0
6	F	96/98 (98%)	71 (74%)	25 (26%)	0	0
7	G	66/71 (93%)	58 (88%)	8 (12%)	5	9
8	H	64/74 (86%)	47 (73%)	17 (27%)	0	0
9	I	44/60 (73%)	26 (59%)	18 (41%)	0	0
10	J	51/52 (98%)	33 (65%)	18 (35%)	0	0
11	K	41/46 (89%)	31 (76%)	10 (24%)	1	0
All	All	1764/1815 (97%)	1379 (78%)	385 (22%)	1	1

All (385) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	18	GLN
1	A	21	ASN
1	A	25	VAL
1	A	29	GLN
1	A	32	GLN
1	A	34	THR
1	A	37	VAL
1	A	42	ASP
1	A	45	SER
1	A	51	LYS
1	A	76	GLU
1	A	81	SER
1	A	90	SER
1	A	99	ILE
1	A	100	LYS
1	A	102	LEU
1	A	104	LYS
1	A	106	LEU
1	A	108	LYS
1	A	127	ILE
1	A	128	GLU
1	A	130	GLU

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Mol	Chain	Res	Type
1	A	131	ARG
1	A	143	THR
1	A	149	VAL
1	A	159	GLN
1	A	163	LEU
1	A	176	LYS
1	A	177	LEU
1	A	183	THR
1	A	186	LEU
1	A	188	ARG
1	A	191	LYS
1	A	203	LEU
1	A	204	GLU
1	A	206	ARG
1	A	207	GLN
1	A	208	LEU
1	A	214	LYS
1	A	219	LEU
1	A	223	TYR
1	A	226	ASP
1	A	230	THR
1	A	244	ARG
1	A	245	GLU
1	A	250	LEU
1	A	255	ILE
1	A	274	ASN
1	A	277	ILE
1	A	300	THR
1	A	302	LYS
1	A	305	GLN
1	A	306	SER
1	A	320	LEU
1	A	323	HIS
1	A	351	GLU
1	A	369	LEU
1	A	370	ASP
1	A	381	ARG
1	A	388	ARG
1	A	389	ARG
1	A	398	ARG
1	A	405	ARG
1	A	406	VAL

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Mol	Chain	Res	Type
1	A	408	ARG
1	A	409	GLU
1	A	413	LYS
1	A	418	GLN
1	A	438	ARG
2	B	17	VAL
2	B	20	HIS
2	B	22	GLN
2	B	24	LEU
2	B	33	LEU
2	B	35	ILE
2	B	38	LEU
2	B	40	ASN
2	B	52	LYS
2	B	69	LEU
2	B	86	THR
2	B	98	VAL
2	B	99	THR
2	B	102	ARG
2	B	109	VAL
2	B	113	ARG
2	B	152	LEU
2	B	154	ASN
2	B	163	LEU
2	B	169	ARG
2	B	170	ASN
2	B	183	ILE
2	B	186	VAL
2	B	189	VAL
2	B	227	ARG
2	B	230	LEU
2	B	232	LEU
2	B	236	LYS
2	B	248	ASN
2	B	251	SER
2	B	257	LEU
2	B	258	VAL
2	B	273	SER
2	B	276	GLN
2	B	290	ASN
2	B	292	THR
2	B	305	GLN

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Mol	Chain	Res	Type
2	B	309	VAL
2	B	328	SER
2	B	344	VAL
2	B	346	THR
2	B	353	SER
2	B	357	VAL
2	B	358	GLN
2	B	361	LYS
2	B	362	ASN
2	B	370	MET
2	B	376	GLU
2	B	384	SER
2	B	391	SER
2	B	396	SER
2	B	397	THR
2	B	409	ASP
2	B	415	LYS
2	B	421	ARG
2	B	422	LYS
2	B	424	MET
3	C	4	ILE
3	C	11	MET
3	C	21	LEU
3	C	42	ILE
3	C	46	LEU
3	C	56	THR
3	C	60	THR
3	C	67	THR
3	C	78	ILE
3	C	79	ILE
3	C	80	ARG
3	C	96	MET
3	C	110	LEU
3	C	120	LEU
3	C	124	MET
3	C	129	MET
3	C	138	MET
3	C	146	ILE
3	C	156	ILE
3	C	158	THR
3	C	164	ILE
3	C	168	PHE

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Mol	Chain	Res	Type
3	C	169	SER
3	C	171	ASP
3	C	174	THR
3	C	175	LEU
3	C	176	THR
3	C	185	LEU
3	C	198	LEU
3	C	212	SER
3	C	217	LYS
3	C	226	ILE
3	C	228	ASP
3	C	242	LEU
3	C	243	VAL
3	C	248	ASP
3	C	249	LEU
3	C	252	ASP
3	C	263	ASN
3	C	264	THR
3	C	268	ILE
3	C	269	LYS
3	C	281	LEU
3	C	282	ARG
3	C	284	ILE
3	C	292	LEU
3	C	298	ILE
3	C	300	ILE
3	C	309	THR
3	C	316	MET
3	C	318	ARG
3	C	320	LEU
3	C	328	LEU
3	C	333	LEU
3	C	336	THR
3	C	343	VAL
3	C	344	GLU
3	C	349	THR
3	C	350	ILE
3	C	360	LEU
3	C	361	LEU
3	C	363	LEU
3	C	365	LEU
3	C	371	THR

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Mol	Chain	Res	Type
3	C	378	LYS
3	C	379	TRP
4	D	1	SER
4	D	2	ASP
4	D	5	LEU
4	D	9	SER
4	D	13	SER
4	D	18	LEU
4	D	24	THR
4	D	27	ARG
4	D	34	LYS
4	D	37	CYS
4	D	40	CYS
4	D	42	SER
4	D	46	VAL
4	D	54	VAL
4	D	55	CYS
4	D	58	GLU
4	D	60	GLU
4	D	62	LYS
4	D	64	LEU
4	D	66	GLU
4	D	68	VAL
4	D	72	ASP
4	D	76	GLU
4	D	79	GLU
4	D	82	MET
4	D	83	ARG
4	D	86	LYS
4	D	91	PHE
4	D	97	ASN
4	D	112	ASP
4	D	114	SER
4	D	116	ILE
4	D	118	ARG
4	D	120	ARG
4	D	121	HIS
4	D	130	LEU
4	D	132	THR
4	D	135	CYS
4	D	139	THR
4	D	143	LEU

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Mol	Chain	Res	Type
4	D	145	GLU
4	D	147	LEU
4	D	153	PHE
4	D	158	ILE
4	D	165	TYR
4	D	166	ASN
4	D	168	VAL
4	D	170	GLU
4	D	179	MET
4	D	180	SER
4	D	203	ARG
4	D	210	LEU
4	D	211	MET
4	D	212	MET
4	D	223	LYS
4	D	224	ARG
4	D	234	LYS
4	D	241	LYS
5	E	5	ILE
5	E	6	LYS
5	E	9	ASP
5	E	19	LEU
5	E	23	LYS
5	E	25	SER
5	E	27	GLU
5	E	29	SER
5	E	43	THR
5	E	44	THR
5	E	52	LYS
5	E	54	VAL
5	E	68	VAL
5	E	69	LEU
5	E	71	MET
5	E	72	SER
5	E	73	LYS
5	E	75	GLU
5	E	77	LYS
5	E	78	LEU
5	E	79	SER
5	E	81	ILE
5	E	85	LYS
5	E	94	LYS

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Mol	Chain	Res	Type
5	E	104	LYS
5	E	108	GLN
5	E	112	VAL
5	E	113	GLU
5	E	115	SER
5	E	116	GLN
5	E	117	LEU
5	E	129	LYS
5	E	152	ASP
5	E	172	ARG
5	E	173	LYS
5	E	181	GLU
5	E	186	GLU
5	E	188	THR
6	F	6	VAL
6	F	7	SER
6	F	10	SER
6	F	11	ARG
6	F	22	ASN
6	F	27	ASN
6	F	29	LEU
6	F	37	ILE
6	F	44	LYS
6	F	47	ILE
6	F	59	VAL
6	F	72	GLN
6	F	73	GLN
6	F	74	ILE
6	F	78	GLU
6	F	82	LYS
6	F	84	GLU
6	F	87	LYS
6	F	88	SER
6	F	90	LEU
6	F	91	GLU
6	F	94	LEU
6	F	99	ARG
6	F	105	GLU
6	F	110	LYS
7	G	14	ILE
7	G	18	LEU
7	G	31	SER

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Mol	Chain	Res	Type
7	G	34	ILE
7	G	36	ASN
7	G	37	VAL
7	G	45	ILE
7	G	53	VAL
8	H	14	VAL
8	H	18	THR
8	H	22	GLU
8	H	27	LEU
8	H	29	LYS
8	H	30	CYS
8	H	37	LEU
8	H	39	LEU
8	H	43	ARG
8	H	47	ARG
8	H	49	GLN
8	H	52	GLU
8	H	60	ASP
8	H	65	ARG
8	H	68	CYS
8	H	72	LYS
8	H	77	LEU
9	I	3	SER
9	I	4	VAL
9	I	7	ARG
9	I	8	SER
9	I	15	LEU
9	I	18	THR
9	I	20	ARG
9	I	22	VAL
9	I	27	ARG
9	I	43	LEU
9	I	44	ASP
9	I	45	LEU
9	I	47	ARG
9	I	48	SER
9	I	49	VAL
9	I	50	LEU
9	I	54	SER
9	I	55	LEU
10	J	1	VAL
10	J	6	THR

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Mol	Chain	Res	Type
10	J	8	ARG
10	J	9	LEU
10	J	12	LEU
10	J	16	ARG
10	J	17	THR
10	J	18	SER
10	J	24	ILE
10	J	25	VAL
10	J	40	ASP
10	J	44	GLU
10	J	46	ILE
10	J	53	LYS
10	J	56	LYS
10	J	58	LYS
10	J	59	TYR
10	J	60	GLU
11	K	3	THR
11	K	6	LEU
11	K	12	GLN
11	K	18	VAL
11	K	20	THR
11	K	22	SER
11	K	24	TRP
11	K	38	TRP
11	K	39	ARG
11	K	49	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	29	GLN
1	A	53	ASN
1	A	69	ASN
1	A	94	HIS
1	A	136	GLN
1	A	173	ASN
1	A	189	HIS
1	A	213	GLN
1	A	215	HIS
1	A	274	ASN
1	A	311	ASN

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Mol	Chain	Res	Type
1	A	323	HIS
1	A	341	GLN
1	A	359	ASN
1	A	418	GLN
2	B	143	GLN
2	B	154	ASN
2	B	162	ASN
2	B	170	ASN
2	B	174	ASN
2	B	218	GLN
2	B	270	ASN
2	B	276	GLN
2	B	305	GLN
2	B	329	GLN
2	B	342	ASN
2	B	343	GLN
2	B	351	ASN
2	B	362	ASN
2	B	385	GLN
3	C	8	HIS
3	C	32	ASN
3	C	74	ASN
3	C	114	ASN
3	C	207	ASN
3	C	352	GLN
4	D	31	GLN
4	D	50	HIS
4	D	166	ASN
5	E	57	GLN
5	E	100	HIS
5	E	108	GLN
6	F	72	GLN
7	G	12	HIS
10	J	54	HIS
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 [i](#)

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$
14	UQ2	C	384	-	23,23,23	2.36	5 (21%)	30,31,31	1.47	6 (20%)
15	FES	E	197	5	0,4,4	-	-	-		
12	HEC	D	242	4	50,50,50	1.25	5 (10%)	68,82,82	1.88	17 (25%)
13	UHD	C	383	-	24,24,24	2.06	8 (33%)	26,31,31	1.98	6 (23%)
12	HEC	C	381	3	50,50,50	1.27	4 (8%)	68,82,82	1.96	20 (29%)
12	HEC	C	382	3	50,50,50	1.27	4 (8%)	68,82,82	1.91	16 (23%)

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
14	UQ2	C	384	-	-	7/15/39/39	0/1/1/1
15	FES	E	197	5	-	-	0/1/1/1
12	HEC	D	242	4	1/1/3/7	8/14/54/54	-
13	UHD	C	383	-	-	8/11/31/31	0/2/2/2
12	HEC	C	381	3	1/1/3/7	4/14/54/54	-
12	HEC	C	382	3	1/1/3/7	9/14/54/54	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	384	UQ2	C6-C5	8.77	1.50	1.35
13	C	383	UHD	C2-S1	4.22	1.79	1.72
12	C	382	HEC	CBA-CGA	-4.18	1.40	1.50
12	C	381	HEC	CBD-CGD	-4.09	1.41	1.50
13	C	383	UHD	C4-C4A	-3.89	1.40	1.48
12	D	242	HEC	CBD-CGD	-3.81	1.41	1.50
14	C	384	UQ2	C3-C2	3.74	1.49	1.36
12	C	381	HEC	CBA-CGA	-3.69	1.42	1.50
12	C	382	HEC	CBD-CGD	-3.57	1.42	1.50
14	C	384	UQ2	C8-C9	3.55	1.41	1.33
13	C	383	UHD	C6-C7A	-3.55	1.41	1.50
13	C	383	UHD	C6-C5	3.54	1.41	1.36
12	D	242	HEC	CBA-CGA	-3.51	1.42	1.50
13	C	383	UHD	C7-S1	3.43	1.78	1.72
13	C	383	UHD	O6-C6	-3.36	1.22	1.33
12	C	381	HEC	C4D-C3D	-2.98	1.40	1.45
13	C	383	UHD	C2-N3	2.81	1.37	1.30
14	C	384	UQ2	C13-C14	2.79	1.40	1.32
12	D	242	HEC	C4D-C3D	-2.72	1.40	1.45
13	C	383	UHD	C7-C7A	-2.45	1.39	1.46
12	C	381	HEC	CHD-C4C	2.43	1.44	1.39
12	C	382	HEC	CHD-C4C	2.41	1.44	1.39
14	C	384	UQ2	C7-C8	2.37	1.54	1.50
12	C	382	HEC	C4D-C3D	-2.36	1.41	1.45
12	D	242	HEC	CHD-C4C	2.29	1.44	1.39
12	D	242	HEC	FE-NA	2.14	2.02	1.95

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	242	HEC	CHB-C4A-NA	5.85	130.82	124.45
12	C	381	HEC	CHB-C4A-NA	5.81	130.78	124.45
12	C	382	HEC	CHA-C1A-NA	4.88	129.77	124.45
12	D	242	HEC	CHA-C1A-NA	4.87	129.76	124.45
12	C	382	HEC	C2A-C1A-NA	-4.82	105.67	110.32
12	C	382	HEC	C4C-CHD-C1D	-4.74	115.10	126.25
12	C	382	HEC	C4A-CHB-C1B	-4.66	116.11	126.02
12	C	381	HEC	C2A-C1A-NA	-4.55	105.94	110.32
13	C	383	UHD	C5-C6-C7A	-4.38	120.72	123.10
12	C	382	HEC	C4A-NA-C1A	4.30	112.82	105.82
12	C	381	HEC	CHA-C1A-NA	4.20	129.02	124.45
13	C	383	UHD	C7A-C7-S1	4.03	129.66	121.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	242	HEC	C2A-C1A-NA	-3.84	106.61	110.32
12	D	242	HEC	CHD-C1D-ND	3.84	129.12	124.37
12	C	381	HEC	C4A-CHB-C1B	-3.82	117.90	126.02
13	C	383	UHD	S1-C2-N3	-3.80	112.82	116.08
14	C	384	UQ2	C5-C6-C1	-3.74	115.98	119.62
12	C	381	HEC	CHC-C4B-NB	3.72	128.97	124.37
13	C	383	UHD	O4-C4A-C4	-3.69	116.80	123.10
12	C	381	HEC	C4C-CHD-C1D	-3.56	117.87	126.25
13	C	383	UHD	C8-C5-C4A	3.56	122.84	116.92
12	C	381	HEC	CHB-C1B-NB	3.54	128.23	124.42
12	C	381	HEC	C1C-CHC-C4B	-3.45	118.13	126.25
12	C	382	HEC	CHB-C4A-NA	3.39	128.14	124.45
12	C	381	HEC	C4A-NA-C1A	3.36	111.31	105.82
12	C	382	HEC	CHD-C1D-ND	3.36	128.52	124.37
12	D	242	HEC	C4C-CHD-C1D	-3.31	118.47	126.25
12	D	242	HEC	CHB-C1B-NB	3.28	127.95	124.42
12	D	242	HEC	C4A-CHB-C1B	-3.20	119.21	126.02
12	D	242	HEC	CHA-C4D-ND	3.09	127.75	124.42
12	D	242	HEC	C4A-NA-C1A	3.08	110.84	105.82
12	C	382	HEC	C4B-NB-C1B	3.07	108.84	105.21
13	C	383	UHD	O7-C7A-C6	2.98	122.36	117.47
14	C	384	UQ2	C10-C9-C11	2.92	120.29	115.23
12	D	242	HEC	CHC-C4B-NB	2.80	127.84	124.37
12	C	381	HEC	CHA-C4D-ND	2.79	127.43	124.42
12	C	382	HEC	C3A-C4A-NA	-2.77	104.51	109.64
14	C	384	UQ2	C8-C7-C6	2.76	118.88	112.08
12	D	242	HEC	C1A-CHA-C4D	-2.68	120.32	126.02
12	C	382	HEC	CAC-C3C-C2C	2.65	131.08	126.89
12	C	382	HEC	C3B-C4B-NB	-2.63	107.29	110.17
12	D	242	HEC	CHC-C1C-NC	2.62	128.61	123.86
12	C	382	HEC	C1C-CHC-C4B	-2.61	120.10	126.25
12	C	381	HEC	CHD-C1D-ND	2.55	127.52	124.37
12	C	381	HEC	CAD-CBD-CGD	-2.54	106.94	113.67
12	D	242	HEC	C1C-CHC-C4B	-2.49	120.38	126.25
12	C	381	HEC	CBB-CAB-C3B	-2.47	105.73	112.42
12	C	381	HEC	CHD-C4C-NC	2.34	128.11	123.86
12	C	382	HEC	C1A-CHA-C4D	-2.32	121.08	126.02
12	C	382	HEC	CBC-CAC-C3C	2.20	118.40	112.42
12	D	242	HEC	CBB-CAB-C3B	2.20	118.38	112.42
14	C	384	UQ2	C6-C5-C4	2.20	120.90	119.17
12	C	381	HEC	CAA-C2A-C3A	-2.18	123.78	127.87
12	C	382	HEC	CAC-C3C-C4C	-2.16	121.94	124.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	382	HEC	CHC-C4B-NB	2.13	127.00	124.37
12	C	381	HEC	O2A-CGA-O1A	-2.12	117.88	123.33
12	C	381	HEC	CHB-C1B-C2B	-2.10	121.71	125.03
12	D	242	HEC	CAC-C3C-C4C	2.09	127.79	124.91
12	D	242	HEC	CHB-C1B-C2B	-2.08	121.74	125.03
14	C	384	UQ2	C11-C9-C8	-2.07	116.52	121.17
12	C	381	HEC	O2A-CGA-CBA	2.06	120.50	114.00
12	C	381	HEC	C3B-C4B-NB	-2.05	107.92	110.17
12	C	381	HEC	C1A-CHA-C4D	-2.03	121.70	126.02
12	D	242	HEC	O2A-CGA-O1A	-2.01	118.15	123.33
14	C	384	UQ2	O1-C1-C2	-2.00	116.79	121.03

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	C	381	HEC	NA
12	C	382	HEC	NA
12	D	242	HEC	NA

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	C	384	UQ2	C1-C6-C7-C8
12	D	242	HEC	C2B-C3B-CAB-CBB
12	D	242	HEC	C4B-C3B-CAB-CBB
12	C	382	HEC	C4C-C3C-CAC-CBC
12	C	382	HEC	C2C-C3C-CAC-CBC
12	D	242	HEC	C3D-CAD-CBD-CGD
12	C	382	HEC	C2D-C3D-CAD-CBD
13	C	383	UHD	C14-C15-C16-C17
13	C	383	UHD	C11-C10-C9-C8
13	C	383	UHD	C10-C11-C12-C13
12	C	382	HEC	C4D-C3D-CAD-CBD
14	C	384	UQ2	C5-C6-C7-C8
12	D	242	HEC	C2A-CAA-CBA-CGA
13	C	383	UHD	C13-C14-C15-C16
13	C	383	UHD	C12-C13-C14-C15
14	C	384	UQ2	C9-C11-C12-C13
12	C	382	HEC	C3D-CAD-CBD-CGD
13	C	383	UHD	C15-C16-C17-C18
13	C	383	UHD	C9-C10-C11-C12
14	C	384	UQ2	C1-C2-O2-CM2

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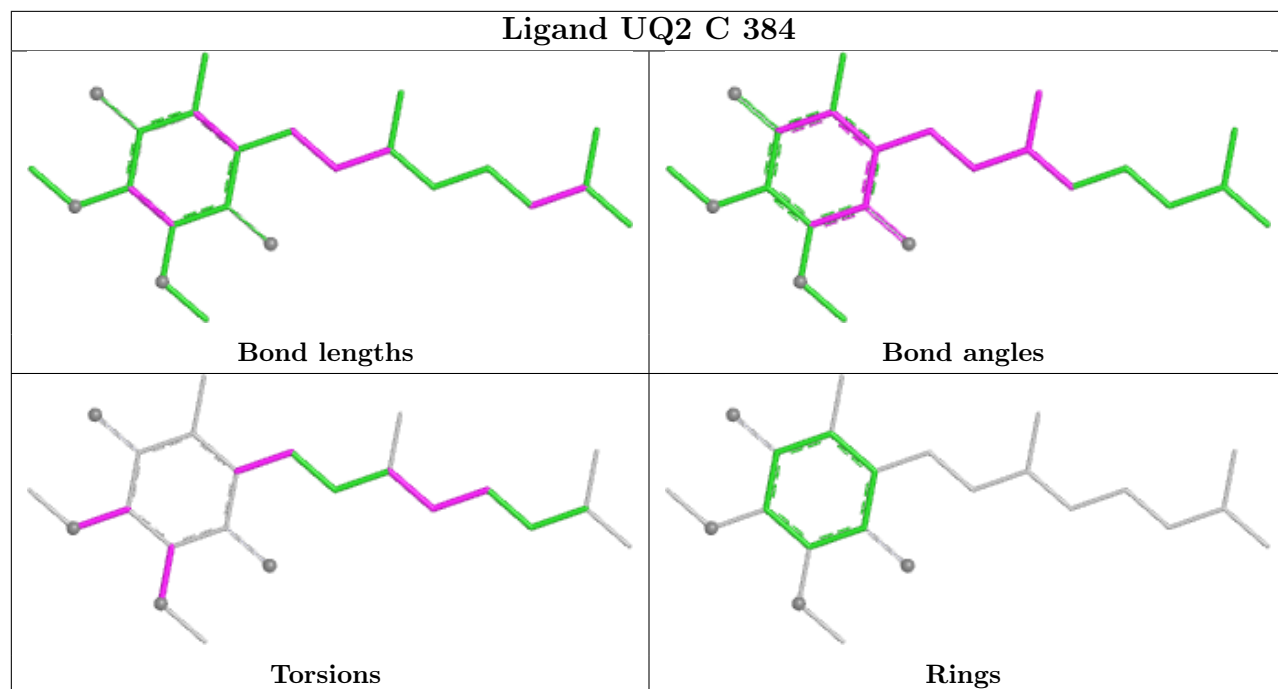
Mol	Chain	Res	Type	Atoms
14	C	384	UQ2	C4-C3-O3-CM3
13	C	383	UHD	C11-C12-C13-C14
12	C	381	HEC	CAD-CBD-CGD-O1D
12	C	382	HEC	CAA-CBA-CGA-O2A
12	D	242	HEC	CAA-CBA-CGA-O1A
12	C	382	HEC	CAD-CBD-CGD-O1D
12	C	382	HEC	CAD-CBD-CGD-O2D
12	D	242	HEC	CAA-CBA-CGA-O2A
12	C	381	HEC	CAD-CBD-CGD-O2D
14	C	384	UQ2	C12-C11-C9-C8
12	C	382	HEC	CAA-CBA-CGA-O1A
12	D	242	HEC	CAD-CBD-CGD-O1D
12	D	242	HEC	CAD-CBD-CGD-O2D
12	C	381	HEC	C2A-CAA-CBA-CGA
14	C	384	UQ2	C12-C11-C9-C10
12	C	381	HEC	CAA-CBA-CGA-O2A

There are no ring outliers.

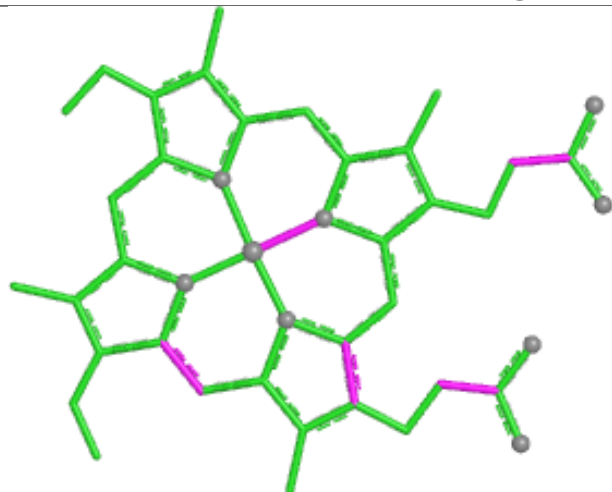
5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	C	384	UQ2	1	0
12	D	242	HEC	4	0
13	C	383	UHD	3	0
12	C	381	HEC	4	0
12	C	382	HEC	7	0

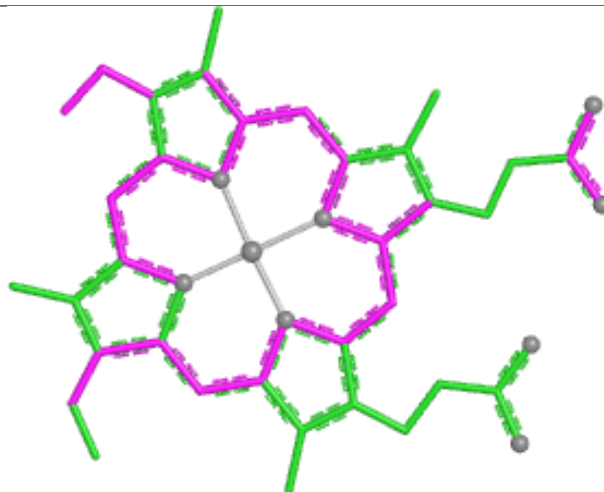
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



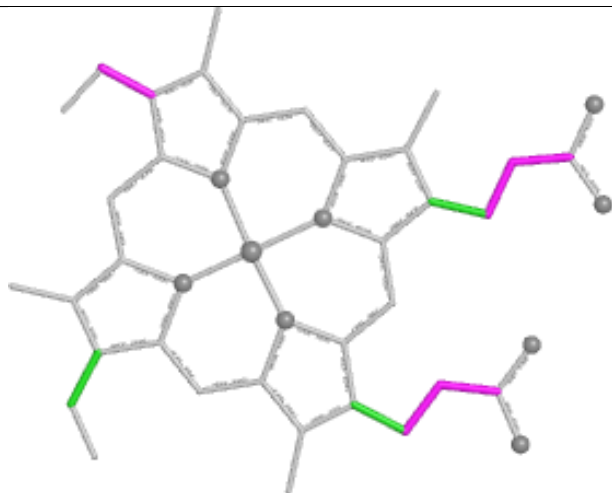
Ligand HEC D 242



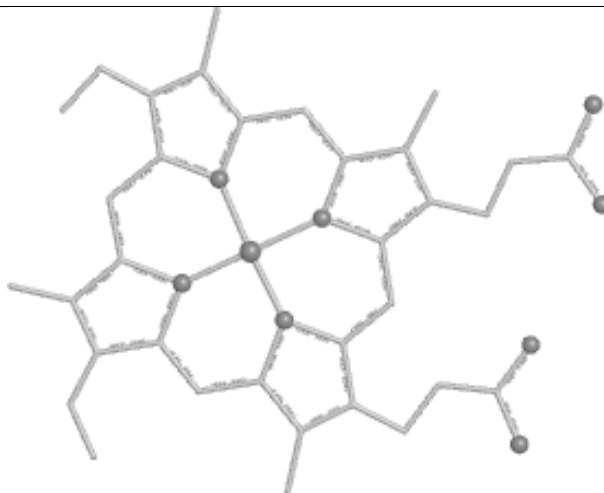
Bond lengths



Bond angles

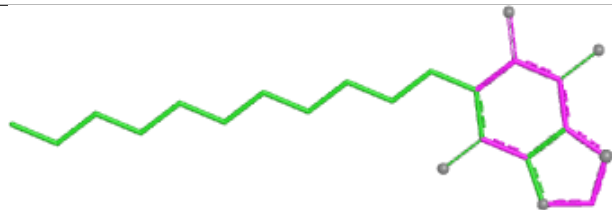


Torsions

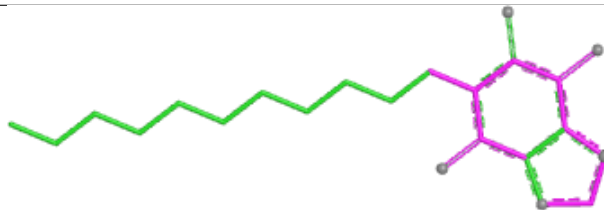


Rings

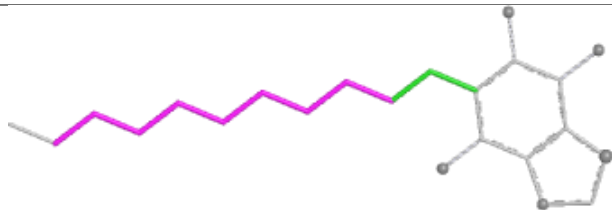
Ligand UHD C 383



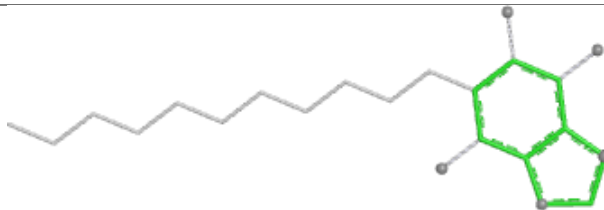
Bond lengths



Bond angles

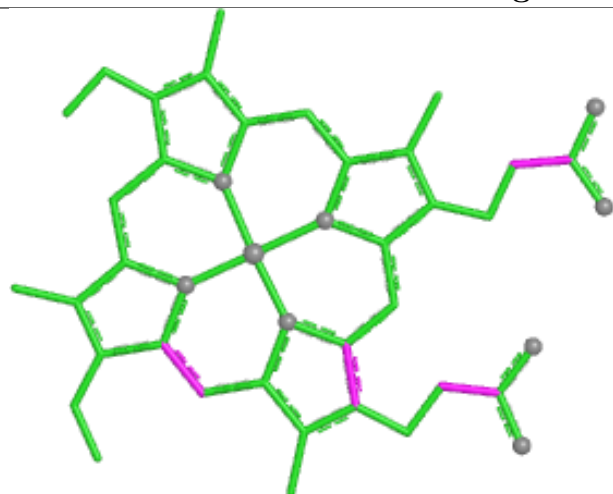


Torsions

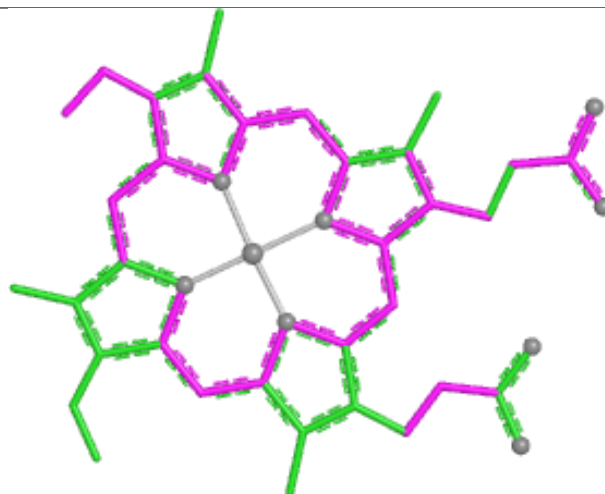


Rings

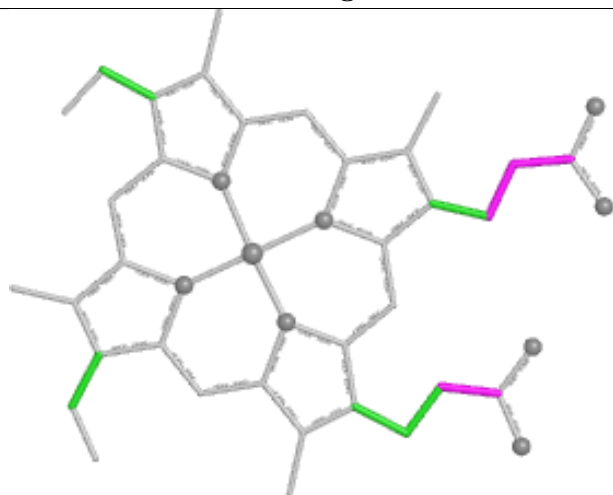
Ligand HEC C 381



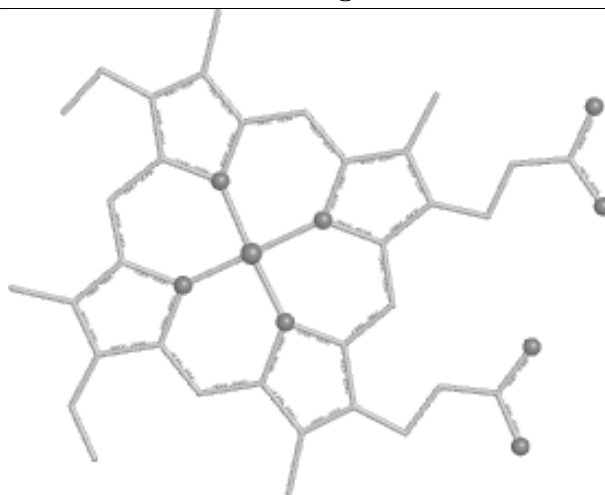
Bond lengths



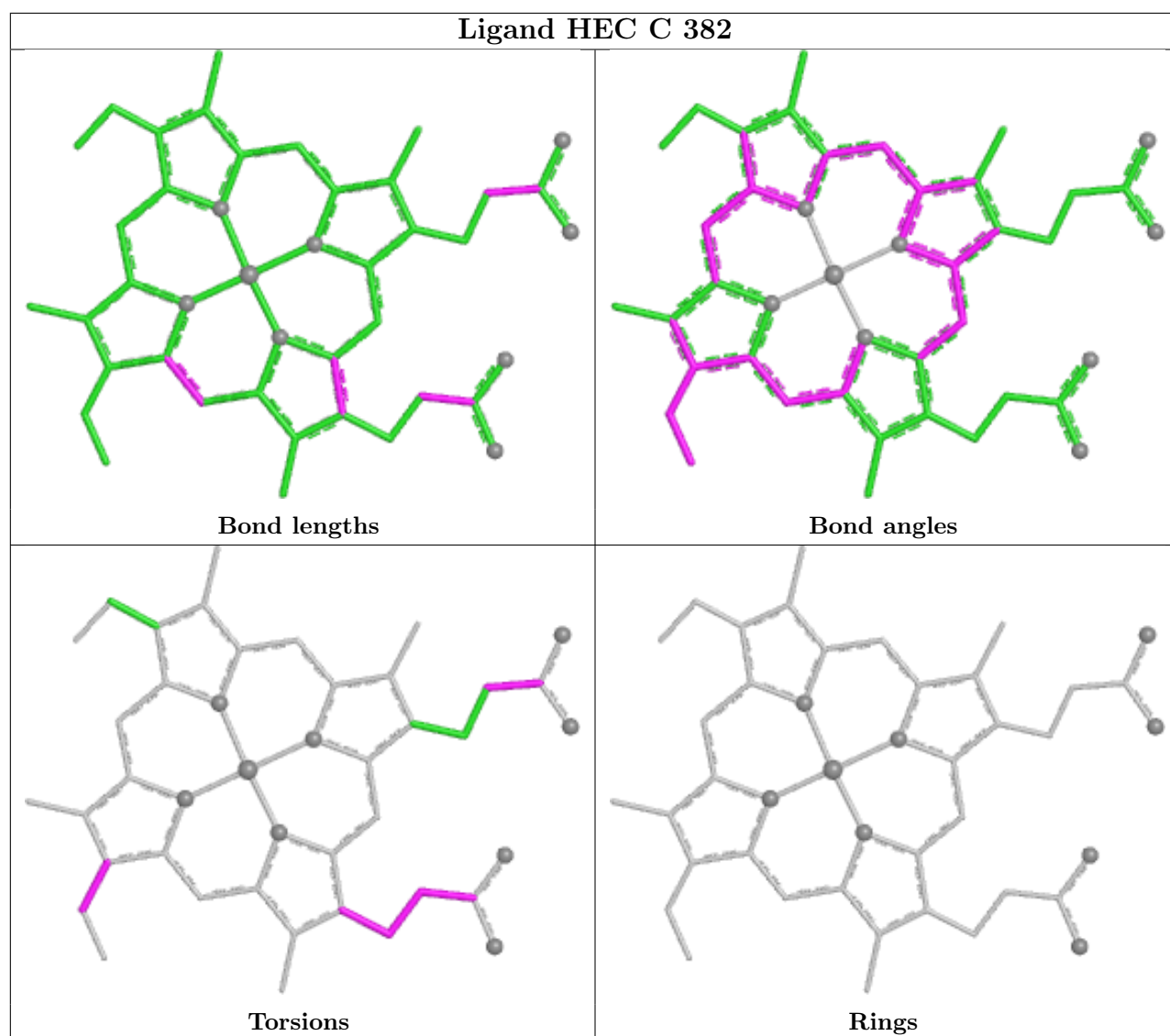
Bond angles



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.