



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 06:43 PM EDT

PDB ID : 1SQP / pdb_00001sqp
Title : Crystal Structure Analysis of Bovine Bcl with Myxothiazol
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 : 2.70 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

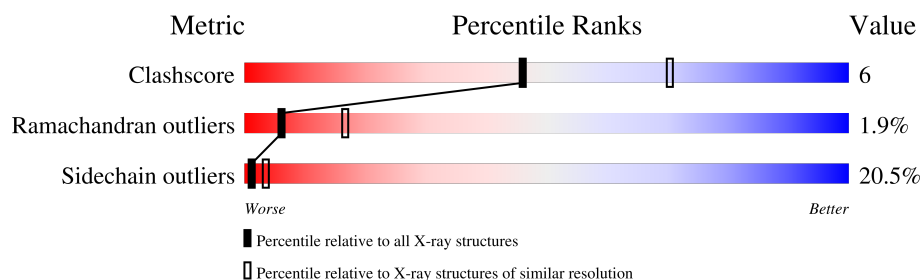
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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	480	69% 22% 7%
2	B	453	72% 17% 7%
3	C	379	69% 25% 5%
4	D	241	64% 29% 5%
5	E	196	64% 32% .
6	F	110	82% 13% 5%
7	G	81	62% 28% 7%
8	H	78	46% 33% 5% 14%

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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	CDL	A	447	X	-	-	-
12	CDL	D	242	X	-	-	-
12	CDL	G	82	X	-	-	-
14	HEC	C	382	X	-	-	-
14	HEC	D	243	X	-	-	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 17274 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
			1919	1225	330	349	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 sub6.

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 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			

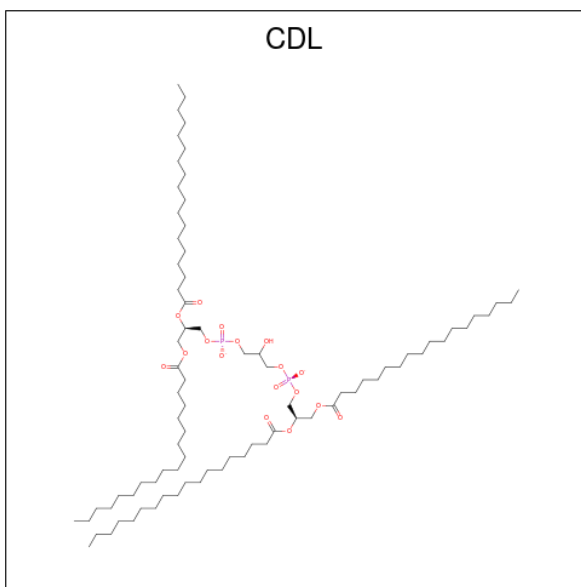
- Molecule 10 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

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

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

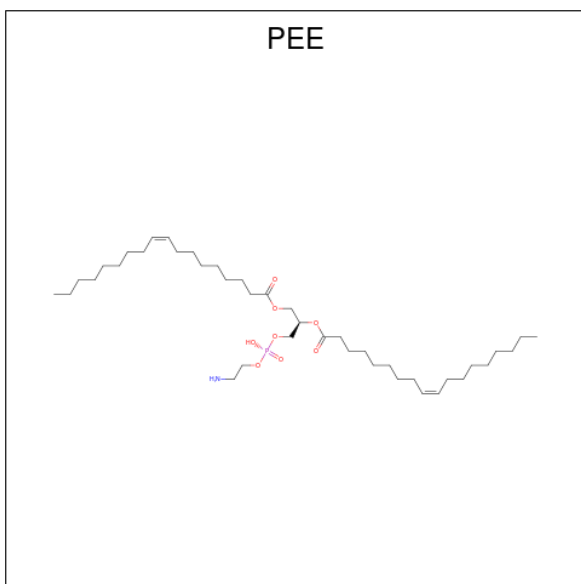
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	53	Total	C	N	O	S	0	0	0
			436	292	78	65	1			

- Molecule 12 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



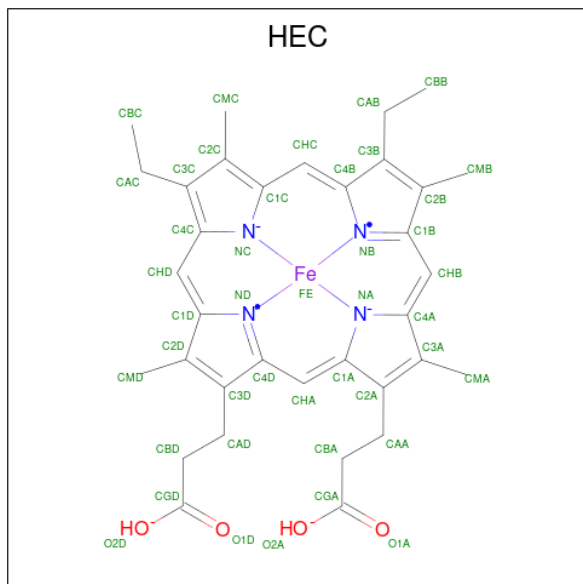
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	O	P	0	0
			64	45	17	2		
12	D	1	Total	C	O	P	0	0
			64	45	17	2		
12	G	1	Total	C	O	P	0	0
			64	45	17	2		

- Molecule 13 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



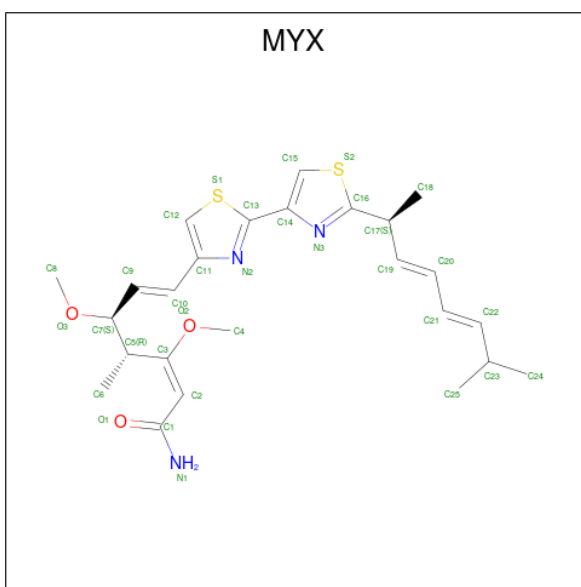
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total 49	C 39	N 1	O 8	P 1	0	0
13	C	1	Total 49	C 39	N 1	O 8	P 1	0	0
13	E	1	Total 49	C 39	N 1	O 8	P 1	0	0

- Molecule 14 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).



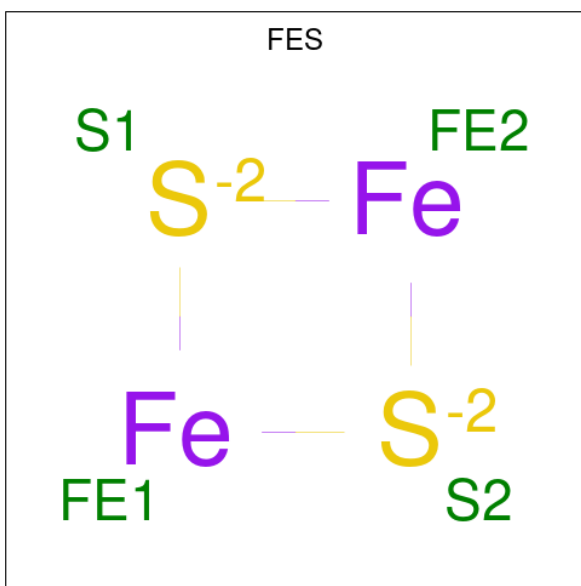
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
14	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 15 is (2Z,6E)-7-{2'-[(2E,4E)-1,6-DIMETHYLHEPTA-2,4-DIENYL]-2,4'-BI-1,3-THIAZOL-4-YL}-3,5-DIMETHOXY-4-METHYLHEPTA-2,6-DIENAMID E (CCD ID: MYX) (formula: C₂₅H₃₃N₃O₃S₂).



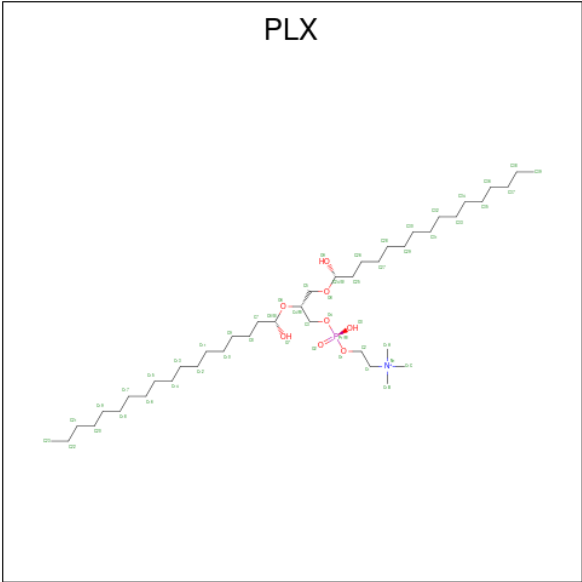
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	N	O	S	0	0
			33	25	3	3	2		

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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

- Molecule 17 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	J	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 18 is water.

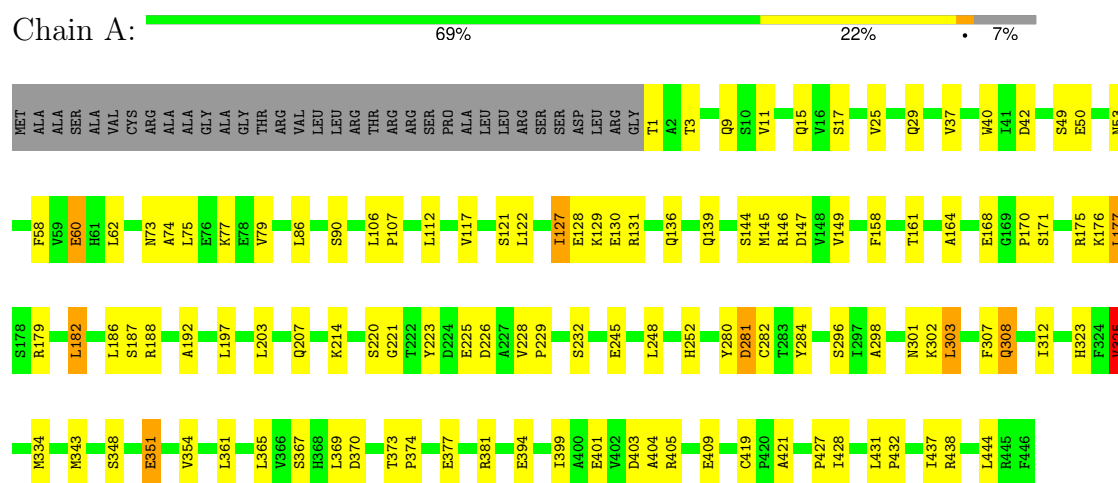
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	51	Total	O	0	0
			51	51		
18	B	84	Total	O	0	0
			84	84		
18	C	36	Total	O	0	0
			36	36		
18	D	11	Total	O	0	0
			11	11		
18	E	2	Total	O	0	0
			2	2		
18	F	15	Total	O	0	0
			15	15		
18	G	11	Total	O	0	0
			11	11		
18	I	2	Total	O	0	0
			2	2		
18	K	3	Total	O	0	0
			3	3		

3 Residue-property plots

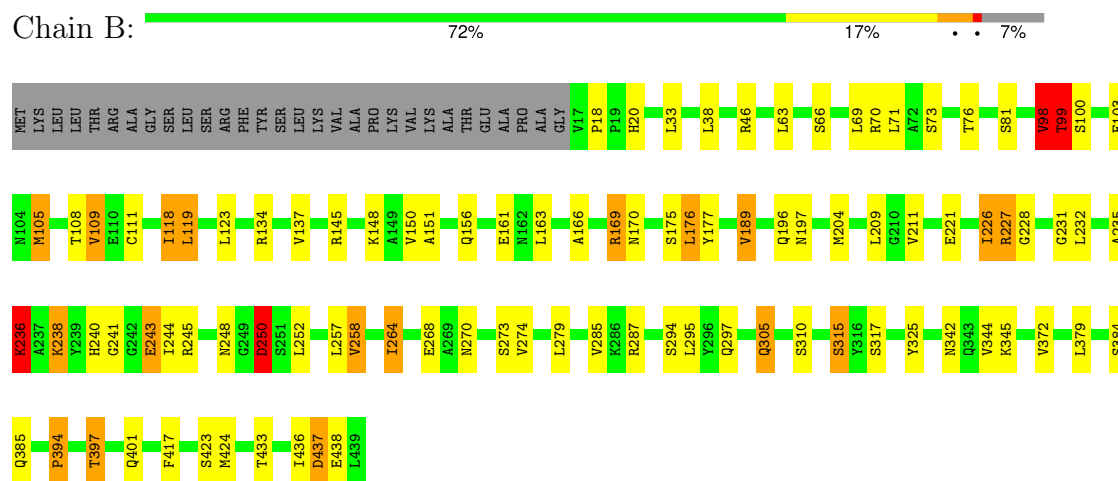
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

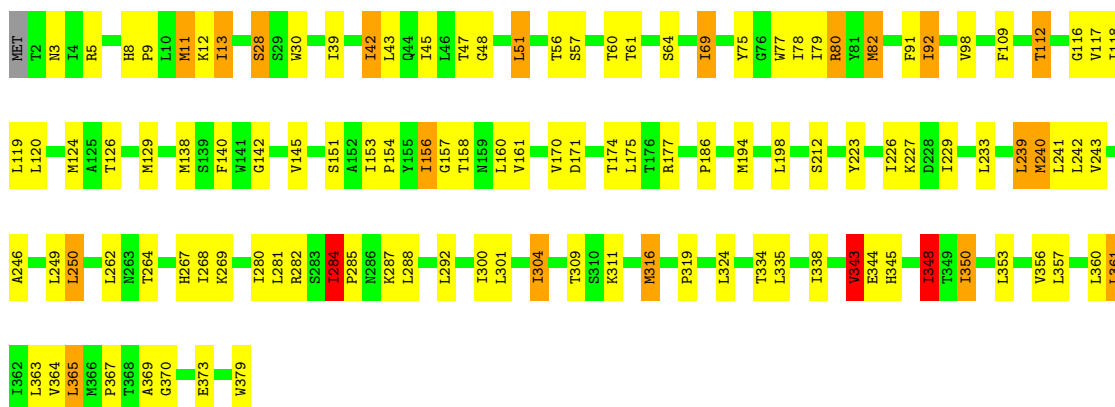


- Molecule 2: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial precursor

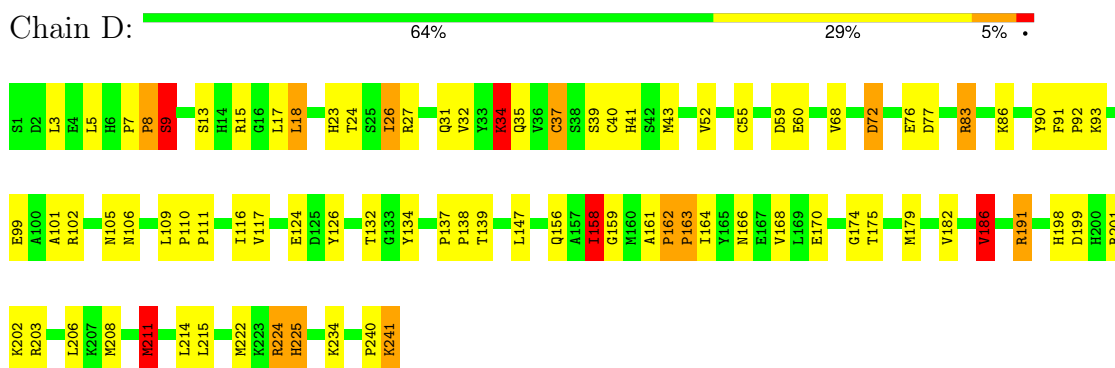


- Molecule 3: Cytochrome b

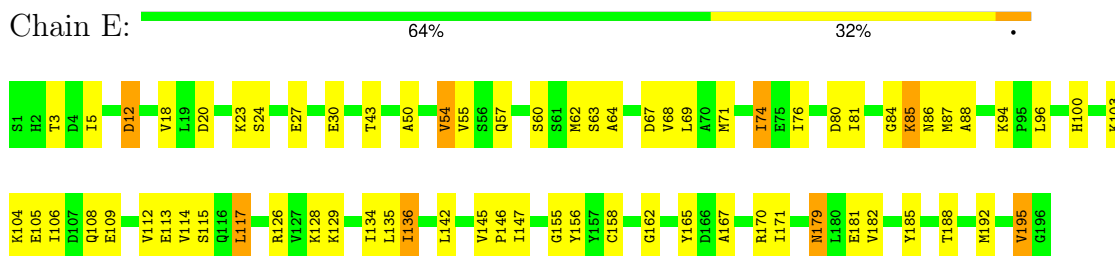




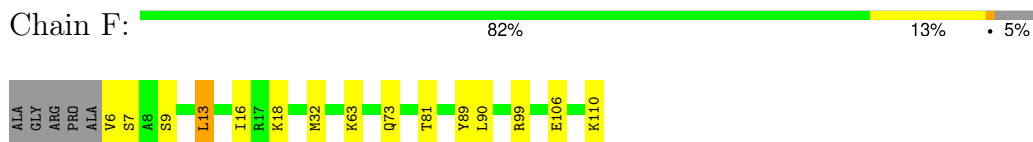
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



- 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: sub6



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

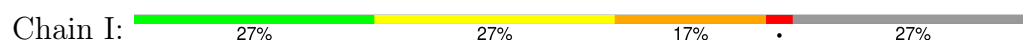




- Molecule 8: Ubiquinol-cytochrome c reductase complex 11 kDa protein



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



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



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



4 Data and refinement statistics

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	153.70Å 153.70Å 596.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.70	Depositor
% Data completeness (in resolution range)	94.1 (40.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.263 , 0.314	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17274	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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: MYX, HEC, CDL, FES, PEE, PLX

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	1.05	8/3531 (0.2%)	1.10	3/4792 (0.1%)
2	B	1.23	12/3232 (0.4%)	1.13	3/4386 (0.1%)
3	C	1.22	16/3100 (0.5%)	1.20	4/4242 (0.1%)
4	D	1.16	6/1978 (0.3%)	1.21	8/2684 (0.3%)
5	E	1.32	10/1553 (0.6%)	1.10	2/2100 (0.1%)
6	F	1.14	1/930 (0.1%)	1.12	1/1246 (0.1%)
7	G	1.33	3/649 (0.5%)	1.16	2/878 (0.2%)
8	H	1.20	5/553 (0.9%)	1.19	0/741
9	I	1.87	8/411 (1.9%)	1.43	3/558 (0.5%)
10	J	1.18	2/515 (0.4%)	1.16	0/696
11	K	1.35	1/452 (0.2%)	1.23	2/618 (0.3%)
All	All	1.21	72/16904 (0.4%)	1.16	28/22941 (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	1
2	B	0	1
6	F	0	1
All	All	0	3

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	34	ILE	CA-CB	12.18	1.60	1.54
2	B	105	MET	SD-CE	-9.31	1.56	1.79
1	A	334	MET	SD-CE	-9.06	1.56	1.79
3	C	11	MET	SD-CE	9.02	2.02	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	26	LEU	CA-C	8.83	1.62	1.52
3	C	92	ILE	CA-CB	8.66	1.65	1.54
4	D	137	PRO	CA-C	8.12	1.56	1.51
8	H	69	VAL	CA-CB	7.92	1.63	1.54
4	D	211	MET	SD-CE	-7.55	1.60	1.79
3	C	348	ILE	CA-CB	7.49	1.63	1.54
9	I	49	VAL	CA-CB	7.16	1.63	1.54
4	D	158	ILE	CA-CB	7.12	1.64	1.54
9	I	17	ALA	CA-C	7.00	1.62	1.52
2	B	18	PRO	CA-C	6.97	1.58	1.52
2	B	189	VAL	CA-CB	6.90	1.63	1.54
9	I	37	THR	CA-CB	6.89	1.64	1.53
3	C	240	MET	SD-CE	-6.84	1.62	1.79
3	C	79	ILE	CA-CB	6.81	1.62	1.54
5	E	55	VAL	CA-CB	6.74	1.62	1.54
5	E	182	VAL	CA-CB	6.67	1.60	1.53
4	D	7	PRO	CA-C	6.59	1.55	1.51
3	C	356	VAL	CA-CB	6.56	1.62	1.54
3	C	156	ILE	CA-CB	6.55	1.62	1.54
9	I	30	VAL	CA-CB	6.52	1.63	1.54
5	E	81	ILE	CA-CB	6.47	1.60	1.53
5	E	171	ILE	CA-CB	6.42	1.63	1.54
9	I	42	VAL	CA-CB	6.36	1.61	1.53
5	E	106	ILE	CA-CB	6.29	1.61	1.54
7	G	53	VAL	CA-CB	6.24	1.61	1.54
4	D	26	ILE	CA-CB	6.23	1.62	1.54
4	D	52	VAL	CA-CB	6.22	1.60	1.54
9	I	45	LEU	CA-C	6.14	1.59	1.53
2	B	264	ILE	CA-CB	6.12	1.60	1.54
6	F	32	MET	SD-CE	6.12	1.94	1.79
3	C	364	VAL	CA-CB	6.10	1.62	1.54
2	B	235	ALA	CA-C	5.92	1.61	1.52
8	H	20	VAL	CA-CB	5.92	1.62	1.54
1	A	127	ILE	CA-CB	5.83	1.63	1.54
11	K	33	VAL	CA-CB	5.77	1.61	1.54
3	C	69	ILE	CA-CB	5.75	1.60	1.54
1	A	421	ALA	CA-CB	-5.74	1.45	1.53
1	A	228	VAL	CA-CB	5.71	1.61	1.54
3	C	343	VAL	CA-CB	5.71	1.62	1.54
2	B	394	PRO	CA-C	5.69	1.57	1.52
5	E	147	ILE	CA-CB	5.66	1.60	1.54
2	B	305	GLN	CA-C	5.62	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	50	THR	CA-CB	5.58	1.61	1.53
2	B	151	ALA	CA-CB	-5.57	1.44	1.53
2	B	226	ILE	CA-CB	5.51	1.60	1.54
10	J	55	ILE	CA-CB	5.50	1.60	1.54
2	B	204	MET	SD-CE	-5.49	1.65	1.79
2	B	372	VAL	CA-CB	5.47	1.60	1.54
5	E	195	VAL	CA-CB	5.46	1.60	1.53
3	C	42	ILE	CA-CB	5.41	1.61	1.54
5	E	114	VAL	CA-CB	5.41	1.61	1.54
1	A	11	VAL	CA-CB	5.40	1.61	1.54
1	A	325	VAL	CA-CB	5.36	1.61	1.54
8	H	14	VAL	CA-CB	5.36	1.60	1.53
3	C	284	ILE	CA-CB	5.36	1.61	1.53
3	C	350	ILE	CA-CB	5.36	1.61	1.54
1	A	79	VAL	CA-CB	5.29	1.60	1.54
5	E	74	ILE	CA-CB	5.29	1.61	1.54
1	A	312	ILE	CA-CB	5.18	1.60	1.54
3	C	153	ILE	CA-CB	5.17	1.60	1.54
3	C	13	ILE	CA-CB	5.17	1.60	1.54
7	G	50	PRO	CA-C	5.13	1.56	1.52
2	B	436	ILE	CA-CB	5.12	1.61	1.54
9	I	44	ASP	CA-C	5.08	1.58	1.53
5	E	5	ILE	CA-CB	5.05	1.61	1.54
10	J	46	ILE	CA-CB	5.05	1.60	1.54
8	H	31	VAL	CA-CB	5.04	1.60	1.54
3	C	243	VAL	CA-CB	5.03	1.60	1.54

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	35	GLN	OE1-CD-NE2	-9.59	113.01	122.60
7	G	50	PRO	N-CA-C	7.36	119.68	110.70
9	I	26	LEU	N-CA-C	6.91	119.50	107.49
4	D	34	LYS	N-CA-C	6.74	118.28	111.07
3	C	345	HIS	N-CA-C	6.42	124.00	109.81
1	A	351	GLU	N-CA-C	6.25	118.09	111.28
1	A	428	ILE	N-CA-C	6.20	118.22	111.77
2	B	73	SER	N-CA-C	6.12	119.84	112.38
4	D	35	GLN	CG-CD-NE2	5.99	125.38	116.40
9	I	36	ALA	N-CA-C	5.56	118.11	109.60
4	D	162	PRO	N-CA-C	5.50	117.41	110.70
4	D	215	LEU	N-CA-C	5.48	117.06	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	89	TYR	N-CA-C	5.44	118.71	111.75
2	B	99	THR	N-CA-C	5.42	117.59	107.99
7	G	45	ILE	N-CA-C	5.35	116.72	110.62
4	D	186	VAL	CB-CA-C	-5.33	105.14	111.97
9	I	52	ARG	N-CA-C	5.27	118.69	107.67
4	D	116	ILE	N-CA-C	5.26	116.73	111.00
11	K	18	VAL	N-CA-C	5.22	120.15	108.88
1	A	192	ALA	N-CA-C	5.21	120.70	113.45
2	B	98	VAL	N-CA-C	5.17	115.42	107.77
5	E	85	LYS	N-CA-C	5.15	116.75	110.41
4	D	137	PRO	N-CA-C	5.11	115.38	110.47
3	C	223	TYR	N-CA-C	5.07	116.49	111.07
3	C	171	ASP	N-CA-C	5.04	116.40	109.29
3	C	91	PHE	N-CA-C	5.03	116.84	111.36
5	E	185	TYR	N-CA-C	5.01	117.28	109.52
11	K	42	LEU	N-CA-C	5.00	118.64	112.54

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	LEU	Peptide
2	B	169	ARG	Mainchain
6	F	99	ARG	Mainchain

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	31	0
2	B	3172	0	3152	45	0
3	C	3003	0	3065	40	0
4	D	1919	0	1869	37	0
5	E	1519	0	1504	14	0
6	F	911	0	902	3	0
7	G	628	0	636	8	0
8	H	548	0	530	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	406	0	437	27	0
10	J	502	0	505	5	0
11	K	436	0	445	12	0
12	A	64	0	72	1	0
12	D	64	0	72	0	0
12	G	64	0	72	2	0
13	A	49	0	75	1	0
13	C	49	0	75	1	0
13	E	49	0	75	3	0
14	C	86	0	64	10	0
14	D	43	0	31	11	0
15	C	33	0	33	1	0
16	E	4	0	0	0	0
17	J	52	0	88	4	0
18	A	51	0	0	0	0
18	B	84	0	0	2	0
18	C	36	0	0	0	0
18	D	11	0	0	0	0
18	E	2	0	0	1	0
18	F	15	0	0	0	0
18	G	11	0	0	1	0
18	I	2	0	0	0	0
18	K	3	0	0	0	0
All	All	17274	0	17058	198	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 6.

All (198) 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:40:CYS:SG	14:D:243:HEC:HAC	1.33	1.68
3:C:11:MET:CE	3:C:11:MET:SD	2.02	1.48
11:K:38:TRP:HE3	11:K:41:ILE:CD1	1.25	1.48
4:D:37:CYS:SG	14:D:243:HEC:CAB	2.06	1.42
11:K:38:TRP:CE3	11:K:41:ILE:CD1	2.04	1.41
4:D:40:CYS:SG	14:D:243:HEC:CAC	2.18	1.30
11:K:38:TRP:CE3	11:K:41:ILE:HD11	1.72	1.19
11:K:38:TRP:HE3	11:K:41:ILE:HD13	1.05	1.14
11:K:38:TRP:CZ3	11:K:41:ILE:HD11	2.15	0.81
11:K:38:TRP:CE3	11:K:41:ILE:HD12	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:38:TRP:CE3	11:K:41:ILE:HD13	1.97	0.78
9:I:4:VAL:HB	9:I:10:PRO:HG2	1.68	0.73
2:B:325:TYR:HB3	9:I:28:PRO:HD2	1.70	0.73
1:A:149:VAL:HG21	1:A:252:HIS:HB3	1.73	0.70
4:D:126:TYR:HE2	14:D:243:HEC:O2A	1.77	0.67
4:D:37:CYS:SG	14:D:243:HEC:C3B	2.82	0.67
2:B:310:SER:HB3	9:I:28:PRO:HD3	1.75	0.66
4:D:117:VAL:HG21	4:D:191:ARG:HA	1.76	0.66
4:D:40:CYS:HG	14:D:243:HEC:HAC	1.51	0.66
3:C:109:PHE:HB3	3:C:112:THR:HG23	1.78	0.65
9:I:9:GLY:HA2	9:I:26:LEU:O	2.01	0.61
2:B:248:ASN:HB3	2:B:250:ASP:HB2	1.83	0.60
4:D:72:ASP:HB2	4:D:83:ARG:HG2	1.85	0.59
4:D:159:GLY:HA3	14:D:243:HEC:HBD2	1.84	0.59
4:D:224:ARG:HD3	7:G:25:ALA:O	2.02	0.59
1:A:58:PHE:HB3	1:A:182:LEU:HD21	1.85	0.59
2:B:385:GLN:HG2	9:I:2:LEU:HD12	1.83	0.59
13:A:448:PEE:H14	17:J:63:PLX:H72	1.84	0.58
2:B:66:SER:HB2	2:B:105:MET:HE2	1.86	0.58
2:B:264:ILE:HD12	2:B:315:SER:HB3	1.84	0.58
14:D:243:HEC:HBB3	14:D:243:HEC:HMB3	1.86	0.58
9:I:34:VAL:HB	9:I:35:PRO:HD3	1.85	0.58
2:B:169:ARG:HD3	2:B:238:LYS:HB3	1.85	0.58
5:E:156:TYR:HB2	5:E:165:TYR:HB2	1.84	0.58
7:G:34:ILE:HA	7:G:37:VAL:HG22	1.85	0.57
4:D:23:HIS:HA	4:D:26:ILE:HD12	1.87	0.56
4:D:147:LEU:HB3	4:D:158:ILE:HA	1.87	0.56
5:E:170:ARG:HA	5:E:179:ASN:HB3	1.86	0.56
2:B:170:ASN:ND2	2:B:236:LYS:O	2.38	0.56
3:C:51:LEU:HD11	3:C:80:ARG:HA	1.88	0.56
5:E:20:ASP:HB3	5:E:23:LYS:HB2	1.87	0.56
3:C:142:GLY:HA2	15:C:383:MYX:H82	1.87	0.56
4:D:40:CYS:HG	14:D:243:HEC:CAC	2.14	0.55
1:A:145:MET:O	1:A:149:VAL:HG23	2.06	0.55
2:B:394:PRO:HG2	2:B:397:THR:HG23	1.89	0.55
3:C:8:HIS:HD2	3:C:11:MET:HG3	1.70	0.55
2:B:99:THR:HG22	9:I:14:VAL:HG13	1.90	0.54
3:C:126:THR:HG21	14:C:382:HEC:HBB3	1.90	0.54
5:E:117:LEU:HD21	5:E:170:ARG:HB3	1.90	0.54
4:D:211:MET:HE1	10:J:31:PHE:CE2	2.43	0.54
2:B:245:ARG:NH2	2:B:433:THR:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:46:LYS:HG2	9:I:47:ARG:N	2.23	0.54
3:C:309:THR:HG21	3:C:367:PRO:O	2.08	0.54
2:B:176:LEU:HD11	9:I:11:PHE:HB3	1.90	0.54
4:D:37:CYS:O	4:D:41:HIS:HB2	2.08	0.53
10:J:10:TYR:HA	10:J:14:PHE:HB2	1.91	0.53
3:C:369:ALA:O	3:C:373:GLU:HG3	2.08	0.53
1:A:351:GLU:H	11:K:12:GLN:NE2	2.07	0.53
2:B:279:LEU:HB3	2:B:295:LEU:HG	1.90	0.53
13:E:197:PEE:H62	17:J:63:PLX:H171	1.89	0.53
2:B:150:VAL:HG11	9:I:47:ARG:HD3	1.91	0.52
2:B:166:ALA:HB2	2:B:244:ILE:HG13	1.91	0.52
1:A:86:LEU:HD23	2:B:285:VAL:HG13	1.90	0.52
3:C:357:LEU:O	3:C:361:LEU:HB2	2.10	0.52
5:E:50:ALA:O	5:E:54:VAL:HG23	2.10	0.52
7:G:9:ARG:HD3	18:G:693:HOH:O	2.08	0.52
9:I:20:ARG:HE	9:I:51:CYS:HA	1.74	0.52
3:C:75:TYR:CD1	5:E:57:GLN:HG2	2.44	0.51
4:D:211:MET:HE1	10:J:31:PHE:HE2	1.76	0.51
5:E:12:ASP:HB2	18:E:674:HOH:O	2.11	0.51
2:B:227:ARG:HH22	2:B:231:GLY:HA2	1.76	0.51
2:B:264:ILE:HG12	9:I:2:LEU:HD23	1.92	0.51
2:B:71:LEU:HD23	9:I:15:LEU:HG	1.93	0.50
2:B:384:SER:HB2	9:I:2:LEU:O	2.12	0.50
6:F:63:LYS:HD3	7:G:13:VAL:HG11	1.93	0.50
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.47	0.50
3:C:343:VAL:HG22	3:C:348:ILE:HG23	1.94	0.50
2:B:161:GLU:HG2	2:B:175:SER:OG	2.11	0.50
3:C:267:HIS:HD2	3:C:269:LYS:HB2	1.76	0.50
1:A:158:PHE:O	1:A:164:ALA:HB2	2.12	0.49
1:A:432:PRO:HB2	1:A:437:ILE:HG13	1.94	0.49
3:C:117:VAL:N	14:C:381:HEC:HBC2	2.27	0.49
1:A:146:ARG:HH12	1:A:308:GLN:HE22	1.60	0.49
1:A:131:ARG:NH2	1:A:177:LEU:O	2.45	0.49
1:A:373:THR:HB	1:A:374:PRO:HD3	1.94	0.48
4:D:134:TYR:CE2	4:D:162:PRO:HB3	2.47	0.48
7:G:24:ARG:HD2	7:G:27:PRO:HA	1.95	0.48
2:B:150:VAL:CG1	9:I:47:ARG:HD3	2.44	0.48
2:B:156:GLN:HG2	9:I:27:ARG:HG3	1.95	0.48
4:D:138:PRO:HB3	8:H:58:LEU:HD13	1.96	0.48
4:D:161:ALA:O	4:D:163:PRO:HD3	2.13	0.48
1:A:62:LEU:HD13	1:A:122:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:LEU:HD12	1:A:432:PRO:HD2	1.96	0.48
2:B:76:THR:HG23	2:B:81:SER:HA	1.94	0.48
4:D:208:MET:HA	13:E:197:PEE:H48	1.96	0.48
10:J:37:GLN:HA	10:J:40:ASP:HB2	1.96	0.48
2:B:243:GLU:HA	2:B:424:MET:O	2.14	0.48
2:B:70:ARG:HG3	2:B:98:VAL:HG22	1.96	0.48
2:B:134:ARG:NH1	18:B:580:HOH:O	2.46	0.48
1:A:280:TYR:HB3	1:A:307:PHE:CE2	2.49	0.47
6:F:9:SER:O	6:F:13:LEU:HG	2.13	0.47
2:B:100:SER:O	9:I:13:PRO:HD2	2.13	0.47
1:A:75:LEU:HD12	1:A:112:LEU:HD22	1.97	0.47
3:C:119:LEU:HB3	14:C:381:HEC:HBB3	1.97	0.47
1:A:354:VAL:HG21	1:A:404:ALA:HA	1.96	0.47
3:C:28:SER:HB3	3:C:30:TRP:H	1.79	0.47
3:C:119:LEU:HD22	14:C:381:HEC:HBB3	1.96	0.47
3:C:309:THR:HG23	3:C:370:GLY:HA3	1.96	0.47
3:C:361:LEU:HA	3:C:365:LEU:HB2	1.95	0.47
10:J:8:ARG:O	10:J:12:LEU:HB2	2.14	0.46
2:B:108:THR:HG21	18:B:556:HOH:O	2.16	0.46
2:B:342:ASN:HD22	2:B:345:LYS:HD2	1.80	0.46
1:A:361:LEU:HD23	1:A:399:ILE:HG12	1.98	0.46
4:D:225:HIS:O	7:G:20:PRO:HB3	2.16	0.46
4:D:222:MET:HE2	5:E:43:THR:HG21	1.98	0.46
3:C:116:GLY:HA2	3:C:119:LEU:HD12	1.97	0.46
1:A:301:ASN:HB2	1:A:303:LEU:HG	1.98	0.46
1:A:325:VAL:HG21	9:I:43:LEU:HD12	1.97	0.46
5:E:87:MET:HE3	5:E:88:ALA:H	1.81	0.46
5:E:84:GLY:H	5:E:100:HIS:HB3	1.81	0.46
4:D:101:ALA:HB1	4:D:110:PRO:HD2	1.98	0.46
3:C:77:TRP:CZ3	4:D:201:ARG:HB3	2.51	0.45
12:G:82:CDL:HA61	12:G:82:CDL:H512	1.98	0.45
1:A:419:CYS:SG	1:A:438:ARG:NH1	2.89	0.45
4:D:32:VAL:O	4:D:37:CYS:SG	2.74	0.45
4:D:240:PRO:HB2	4:D:241:LYS:HD3	1.99	0.45
9:I:14:VAL:HB	9:I:22:VAL:HG23	1.99	0.45
11:K:38:TRP:C	11:K:40:LEU:N	2.74	0.45
2:B:344:VAL:HG11	2:B:417:PHE:CD2	2.52	0.45
2:B:325:TYR:HB3	9:I:28:PRO:CD	2.42	0.45
6:F:13:LEU:HA	6:F:16:ILE:HD12	1.98	0.45
12:A:447:CDL:H111	12:A:447:CDL:HB61	1.99	0.45
3:C:186:PRO:HG3	14:C:382:HEC:HBB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:324:LEU:HD12	3:C:369:ALA:HB2	1.99	0.45
4:D:32:VAL:HB	4:D:186:VAL:HG13	1.97	0.45
2:B:111:CYS:HB3	2:B:119:LEU:HD13	1.99	0.45
1:A:252:HIS:NE2	9:I:43:LEU:HG	2.32	0.44
4:D:40:CYS:SG	14:D:243:HEC:C3C	3.00	0.44
9:I:43:LEU:HA	9:I:46:LYS:HB3	1.98	0.44
11:K:39:ARG:HD3	11:K:39:ARG:H	1.82	0.44
1:A:298:ALA:HA	1:A:303:LEU:HB2	2.00	0.44
2:B:394:PRO:HG2	2:B:397:THR:CG2	2.47	0.44
1:A:248:LEU:O	1:A:427:PRO:HG3	2.17	0.44
4:D:110:PRO:HA	4:D:111:PRO:HD3	1.84	0.44
3:C:51:LEU:HD23	3:C:69:ILE:HD13	1.99	0.44
3:C:246:ALA:HB1	3:C:249:LEU:HB2	2.00	0.44
3:C:186:PRO:HG2	14:C:382:HEC:HMC3	1.99	0.44
11:K:38:TRP:O	11:K:39:ARG:C	2.60	0.44
9:I:27:ARG:HA	9:I:28:PRO:HD2	1.98	0.43
1:A:53:ASN:HB3	1:A:170:PRO:HD2	2.01	0.43
4:D:166:ASN:HB3	8:H:13:LEU:HD22	2.01	0.43
3:C:319:PRO:HB3	7:G:47:ARG:HH11	1.83	0.43
4:D:166:ASN:HD22	8:H:13:LEU:HD22	1.84	0.43
3:C:47:THR:HG21	3:C:82:MET:HB3	2.01	0.43
3:C:250:LEU:HD22	3:C:250:LEU:H	1.84	0.43
2:B:118:ILE:H	2:B:118:ILE:HG13	1.72	0.43
1:A:144:SER:HA	9:I:42:VAL:HG11	2.01	0.43
3:C:284:ILE:HA	3:C:285:PRO:HD3	1.93	0.43
3:C:98:VAL:HG22	14:C:381:HEC:HAC	2.01	0.42
12:G:82:CDL:H311	12:G:82:CDL:H121	2.00	0.42
2:B:103:GLU:OE1	2:B:317:SER:N	2.52	0.42
3:C:11:MET:CE	3:C:11:MET:CG	2.93	0.42
4:D:225:HIS:CD2	7:G:20:PRO:HB2	2.53	0.42
2:B:99:THR:HB	9:I:14:VAL:HG22	2.02	0.42
2:B:325:TYR:CB	9:I:28:PRO:HD2	2.44	0.42
3:C:239:LEU:HD13	3:C:240:MET:HG2	2.01	0.42
3:C:280:ILE:HG13	3:C:335:LEU:HD22	2.01	0.42
5:E:136:ILE:H	5:E:136:ILE:HG13	1.73	0.42
1:A:25:VAL:HG13	1:A:197:LEU:HD23	2.00	0.42
1:A:106:LEU:N	1:A:107:PRO:HD2	2.34	0.42
1:A:281:ASP:HB3	1:A:284:TYR:CE1	2.55	0.42
5:E:145:VAL:HA	5:E:146:PRO:HD3	1.95	0.42
9:I:20:ARG:HD2	9:I:48:SER:HB2	2.02	0.42
5:E:109:GLU:HG3	5:E:167:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:GLU:OE1	2:B:287:ARG:NH2	2.49	0.41
2:B:258:VAL:HG12	2:B:423:SER:HB2	2.01	0.41
3:C:301:LEU:HA	3:C:304:ILE:HD12	2.02	0.41
4:D:8:PRO:HB2	4:D:9:SER:H	1.69	0.41
5:E:136:ILE:HD12	5:E:181:GLU:HB3	2.01	0.41
3:C:316:MET:HE2	13:C:380:PEE:H11	2.02	0.41
17:J:63:PLX:H1C2	17:J:63:PLX:H21	1.73	0.41
2:B:241:GLY:HA2	2:B:423:SER:OG	2.20	0.41
4:D:31:GLN:HA	4:D:34:LYS:HB3	2.01	0.41
1:A:158:PHE:HB3	1:A:161:THR:OG1	2.21	0.41
2:B:148:LYS:HG3	2:B:177:TYR:HB3	2.03	0.41
3:C:140:PHE:CE1	3:C:170:VAL:O	2.74	0.41
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.97	0.41
4:D:147:LEU:HD13	4:D:158:ILE:HG13	2.01	0.41
11:K:45:VAL:HA	11:K:46:PRO:HD3	1.88	0.41
2:B:270:ASN:O	2:B:274:VAL:HG23	2.22	0.40
3:C:116:GLY:C	14:C:381:HEC:HBC2	2.46	0.40
3:C:240:MET:SD	13:E:197:PEE:H17	2.61	0.40
3:C:116:GLY:O	14:C:381:HEC:HMC3	2.21	0.40
1:A:444:LEU:HD22	17:J:63:PLX:H52	2.04	0.40
2:B:109:VAL:HG22	2:B:119:LEU:HD23	2.04	0.40
2:B:156:GLN:H	2:B:156:GLN:NE2	2.20	0.40
3:C:48:GLY:C	14:C:382:HEC:HBC2	2.46	0.40
4:D:163:PRO:HG2	14:D:243:HEC:HMC1	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	444/480 (92%)	418 (94%)	20 (4%)	6 (1%)	9 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	421/453 (93%)	390 (93%)	27 (6%)	4 (1%)	12	32
3	C	376/379 (99%)	353 (94%)	19 (5%)	4 (1%)	11	29
4	D	239/241 (99%)	211 (88%)	21 (9%)	7 (3%)	3	9
5	E	194/196 (99%)	162 (84%)	29 (15%)	3 (2%)	8	22
6	F	103/110 (94%)	98 (95%)	5 (5%)	0	100	100
7	G	73/81 (90%)	66 (90%)	5 (7%)	2 (3%)	4	10
8	H	65/78 (83%)	58 (89%)	5 (8%)	2 (3%)	3	8
9	I	55/78 (70%)	31 (56%)	16 (29%)	8 (14%)	0	0
10	J	59/62 (95%)	50 (85%)	7 (12%)	2 (3%)	3	7
11	K	51/56 (91%)	43 (84%)	7 (14%)	1 (2%)	6	16
All	All	2080/2214 (94%)	1880 (90%)	161 (8%)	39 (2%)	6	17

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	250	ASP
3	C	154	PRO
4	D	8	PRO
7	G	73	ASN
9	I	29	LEU
10	J	56	LYS
11	K	52	PHE
1	A	50	GLU
1	A	220	SER
2	B	437	ASP
3	C	157	GLY
4	D	18	LEU
5	E	155	GLY
8	H	48	SER
9	I	8	SER
9	I	50	LEU
2	B	236	LYS
4	D	158	ILE
4	D	198	HIS
5	E	64	ALA
9	I	9	GLY
10	J	4	THR
1	A	74	ALA

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Mol	Chain	Res	Type
1	A	282	CYS
3	C	9	PRO
8	H	13	LEU
9	I	27	ARG
9	I	51	CYS
1	A	229	PRO
3	C	343	VAL
4	D	9	SER
4	D	163	PRO
9	I	41	PRO
4	D	174	GLY
2	B	228	GLY
9	I	40	SER
1	A	221	GLY
5	E	162	GLY
7	G	74	PRO

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	370/394 (94%)	312 (84%)	58 (16%)	2	7
2	B	332/355 (94%)	288 (87%)	44 (13%)	4	10
3	C	326/327 (100%)	256 (78%)	70 (22%)	1	3
4	D	206/206 (100%)	155 (75%)	51 (25%)	1	2
5	E	168/168 (100%)	127 (76%)	41 (24%)	1	2
6	F	96/99 (97%)	87 (91%)	9 (9%)	8	21
7	G	66/71 (93%)	54 (82%)	12 (18%)	2	5
8	H	64/74 (86%)	36 (56%)	28 (44%)	0	0
9	I	44/60 (73%)	30 (68%)	14 (32%)	0	1
10	J	51/52 (98%)	29 (57%)	22 (43%)	0	0
11	K	42/45 (93%)	29 (69%)	13 (31%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1765/1851 (95%)	1403 (80%)	362 (20%)	1 3

All (362) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	3	THR
1	A	9	GLN
1	A	15	GLN
1	A	17	SER
1	A	29	GLN
1	A	37	VAL
1	A	42	ASP
1	A	49	SER
1	A	60	GLU
1	A	73	ASN
1	A	77	LYS
1	A	90	SER
1	A	117	VAL
1	A	121	SER
1	A	127	ILE
1	A	128	GLU
1	A	129	LYS
1	A	130	GLU
1	A	136	GLN
1	A	139	GLN
1	A	147	ASP
1	A	168	GLU
1	A	171	SER
1	A	175	ARG
1	A	176	LYS
1	A	177	LEU
1	A	179	ARG
1	A	182	LEU
1	A	186	LEU
1	A	187	SER
1	A	188	ARG
1	A	203	LEU
1	A	207	GLN
1	A	214	LYS
1	A	223	TYR
1	A	225	GLU

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Mol	Chain	Res	Type
1	A	226	ASP
1	A	232	SER
1	A	245	GLU
1	A	281	ASP
1	A	296	SER
1	A	302	LYS
1	A	308	GLN
1	A	323	HIS
1	A	325	VAL
1	A	343	MET
1	A	348	SER
1	A	365	LEU
1	A	367	SER
1	A	369	LEU
1	A	370	ASP
1	A	381	ARG
1	A	394	GLU
1	A	401	GLU
1	A	403	ASP
1	A	405	ARG
1	A	409	GLU
2	B	20	HIS
2	B	33	LEU
2	B	38	LEU
2	B	46	ARG
2	B	63	LEU
2	B	69	LEU
2	B	98	VAL
2	B	99	THR
2	B	109	VAL
2	B	118	ILE
2	B	119	LEU
2	B	123	LEU
2	B	137	VAL
2	B	145	ARG
2	B	163	LEU
2	B	176	LEU
2	B	189	VAL
2	B	196	GLN
2	B	197	ASN
2	B	209	LEU
2	B	211	VAL

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Mol	Chain	Res	Type
2	B	221	GLU
2	B	226	ILE
2	B	227	ARG
2	B	232	LEU
2	B	236	LYS
2	B	238	LYS
2	B	240	HIS
2	B	243	GLU
2	B	250	ASP
2	B	252	LEU
2	B	257	LEU
2	B	258	VAL
2	B	268	GLU
2	B	273	SER
2	B	294	SER
2	B	297	GLN
2	B	305	GLN
2	B	315	SER
2	B	379	LEU
2	B	397	THR
2	B	401	GLN
2	B	437	ASP
2	B	438	GLU
3	C	3	ASN
3	C	5	ARG
3	C	12	LYS
3	C	13	ILE
3	C	28	SER
3	C	39	ILE
3	C	42	ILE
3	C	43	LEU
3	C	45	ILE
3	C	51	LEU
3	C	56	THR
3	C	57	SER
3	C	60	THR
3	C	61	THR
3	C	64	SER
3	C	78	ILE
3	C	80	ARG
3	C	82	MET
3	C	92	ILE

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Mol	Chain	Res	Type
3	C	112	THR
3	C	118	ILE
3	C	120	LEU
3	C	124	MET
3	C	129	MET
3	C	138	MET
3	C	145	VAL
3	C	151	SER
3	C	156	ILE
3	C	158	THR
3	C	160	LEU
3	C	161	VAL
3	C	174	THR
3	C	175	LEU
3	C	177	ARG
3	C	194	MET
3	C	198	LEU
3	C	212	SER
3	C	226	ILE
3	C	227	LYS
3	C	229	ILE
3	C	233	LEU
3	C	239	LEU
3	C	241	LEU
3	C	242	LEU
3	C	250	LEU
3	C	262	LEU
3	C	264	THR
3	C	268	ILE
3	C	281	LEU
3	C	282	ARG
3	C	284	ILE
3	C	287	LYS
3	C	288	LEU
3	C	292	LEU
3	C	300	ILE
3	C	304	ILE
3	C	311	LYS
3	C	316	MET
3	C	334	THR
3	C	338	ILE
3	C	343	VAL

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Mol	Chain	Res	Type
3	C	344	GLU
3	C	348	ILE
3	C	350	ILE
3	C	353	LEU
3	C	360	LEU
3	C	361	LEU
3	C	363	LEU
3	C	365	LEU
3	C	379	TRP
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	18	LEU
4	D	24	THR
4	D	27	ARG
4	D	34	LYS
4	D	37	CYS
4	D	39	SER
4	D	43	MET
4	D	55	CYS
4	D	59	ASP
4	D	60	GLU
4	D	68	VAL
4	D	72	ASP
4	D	76	GLU
4	D	77	ASP
4	D	83	ARG
4	D	86	LYS
4	D	90	TYR
4	D	93	LYS
4	D	99	GLU
4	D	102	ARG
4	D	105	ASN
4	D	106	ASN
4	D	109	LEU
4	D	124	GLU
4	D	132	THR
4	D	139	THR
4	D	156	GLN

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Mol	Chain	Res	Type
4	D	164	ILE
4	D	168	VAL
4	D	170	GLU
4	D	175	THR
4	D	179	MET
4	D	182	VAL
4	D	186	VAL
4	D	191	ARG
4	D	199	ASP
4	D	202	LYS
4	D	203	ARG
4	D	206	LEU
4	D	211	MET
4	D	214	LEU
4	D	224	ARG
4	D	225	HIS
4	D	234	LYS
4	D	241	LYS
5	E	3	THR
5	E	12	ASP
5	E	18	VAL
5	E	24	SER
5	E	27	GLU
5	E	30	GLU
5	E	54	VAL
5	E	60	SER
5	E	62	MET
5	E	63	SER
5	E	67	ASP
5	E	68	VAL
5	E	69	LEU
5	E	71	MET
5	E	74	ILE
5	E	76	ILE
5	E	80	ASP
5	E	85	LYS
5	E	86	ASN
5	E	94	LYS
5	E	96	LEU
5	E	103	LYS
5	E	104	LYS
5	E	105	GLU

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Mol	Chain	Res	Type
5	E	108	GLN
5	E	112	VAL
5	E	113	GLU
5	E	115	SER
5	E	117	LEU
5	E	126	ARG
5	E	128	LYS
5	E	129	LYS
5	E	134	ILE
5	E	135	LEU
5	E	136	ILE
5	E	142	LEU
5	E	158	CYS
5	E	179	ASN
5	E	188	THR
5	E	192	MET
5	E	195	VAL
6	F	6	VAL
6	F	7	SER
6	F	13	LEU
6	F	18	LYS
6	F	73	GLN
6	F	81	THR
6	F	90	LEU
6	F	106	GLU
6	F	110	LYS
7	G	2	ARG
7	G	3	GLN
7	G	18	LEU
7	G	32	LYS
7	G	46	LEU
7	G	53	VAL
7	G	60	THR
7	G	64	GLN
7	G	67	GLU
7	G	70	LYS
7	G	71	ARG
7	G	72	LYS
8	H	13	LEU
8	H	14	VAL
8	H	18	THR
8	H	21	ARG

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Mol	Chain	Res	Type
8	H	22	GLU
8	H	27	LEU
8	H	28	GLU
8	H	30	CYS
8	H	31	VAL
8	H	32	LYS
8	H	34	ARG
8	H	35	GLU
8	H	36	ARG
8	H	38	GLU
8	H	42	GLU
8	H	43	ARG
8	H	50	THR
8	H	55	THR
8	H	56	GLU
8	H	58	LEU
8	H	62	LEU
8	H	65	ARG
8	H	68	CYS
8	H	71	HIS
8	H	72	LYS
8	H	73	LEU
8	H	77	LEU
8	H	78	LYS
9	I	2	LEU
9	I	15	LEU
9	I	16	SER
9	I	20	ARG
9	I	22	VAL
9	I	26	LEU
9	I	27	ARG
9	I	28	PRO
9	I	43	LEU
9	I	45	LEU
9	I	46	LYS
9	I	50	LEU
9	I	52	ARG
9	I	55	LEU
10	J	1	VAL
10	J	4	THR
10	J	9	LEU
10	J	12	LEU

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Mol	Chain	Res	Type
10	J	15	ARG
10	J	16	ARG
10	J	18	SER
10	J	25	VAL
10	J	26	VAL
10	J	30	PHE
10	J	36	ASP
10	J	37	GLN
10	J	42	ILE
10	J	44	GLU
10	J	45	HIS
10	J	48	GLU
10	J	53	LYS
10	J	55	ILE
10	J	56	LYS
10	J	58	LYS
10	J	59	TYR
10	J	60	GLU
11	K	1	MET
11	K	2	LEU
11	K	6	LEU
11	K	9	ARG
11	K	13	LEU
11	K	18	VAL
11	K	20	THR
11	K	38	TRP
11	K	39	ARG
11	K	40	LEU
11	K	43	ASP
11	K	44	TRP
11	K	51	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	73	ASN
1	A	119	ASN
1	A	207	GLN
1	A	215	HIS
1	A	264	HIS
1	A	311	ASN

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Mol	Chain	Res	Type
1	A	328	HIS
1	A	339	GLN
1	A	368	HIS
2	B	125	ASN
2	B	141	GLN
2	B	162	ASN
2	B	170	ASN
2	B	174	ASN
2	B	197	ASN
2	B	248	ASN
2	B	329	GLN
2	B	342	ASN
2	B	343	GLN
2	B	432	HIS
3	C	8	HIS
3	C	74	ASN
3	C	114	ASN
3	C	267	HIS
3	C	286	ASN
4	D	31	GLN
4	D	35	GLN
4	D	97	ASN
4	D	105	ASN
4	D	121	HIS
4	D	225	HIS
5	E	57	GLN
5	E	161	HIS
6	F	73	GLN
7	G	3	GLN
9	I	31	GLN
11	K	12	GLN
11	K	49	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](#)

12 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	CDL	D	242	-	63,63,99	1.73	9 (14%)	69,75,111	1.61	7 (10%)
13	PEE	E	197	-	48,48,50	1.57	6 (12%)	51,53,55	1.40	4 (7%)
14	HEC	C	381	3	50,50,50	1.27	5 (10%)	68,82,82	1.97	20 (29%)
15	MYX	C	383	-	30,34,34	2.38	5 (16%)	32,45,45	1.92	9 (28%)
14	HEC	C	382	3	50,50,50	1.40	7 (14%)	68,82,82	1.81	13 (19%)
12	CDL	A	447	-	63,63,99	1.70	8 (12%)	69,75,111	1.65	8 (11%)
13	PEE	C	380	-	48,48,50	1.56	6 (12%)	51,53,55	1.42	6 (11%)
16	FES	E	198	5	0,4,4	-	-	-	-	-
13	PEE	A	448	-	48,48,50	1.63	6 (12%)	51,53,55	1.52	5 (9%)
14	HEC	D	243	4	50,50,50	1.45	7 (14%)	68,82,82	1.92	16 (23%)
12	CDL	G	82	-	63,63,99	1.78	8 (12%)	69,75,111	1.74	10 (14%)
17	PLX	J	63	-	51,51,51	0.77	2 (3%)	53,59,59	0.66	0

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	CDL	D	242	-	1/1/9/9	44/74/74/110	-
13	PEE	E	197	-	-	19/52/52/54	-
14	HEC	C	381	3	-	4/14/54/54	-
15	MYX	C	383	-	-	0/34/36/36	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEC	C	382	3	1/1/3/7	8/14/54/54	-
12	CDL	A	447	-	1/1/9/9	39/74/74/110	-
13	PEE	C	380	-	-	24/52/52/54	-
16	FES	E	198	5	-	-	0/1/1/1
13	PEE	A	448	-	-	29/52/52/54	-
14	HEC	D	243	4	1/1/3/7	8/14/54/54	-
12	CDL	G	82	-	1/1/9/9	42/74/74/110	-
17	PLX	J	63	-	-	36/55/55/55	-

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	383	MYX	C16-N3	6.80	1.45	1.30
15	C	383	MYX	C13-N2	6.41	1.44	1.31
15	C	383	MYX	O2-C3	6.15	1.47	1.35
12	G	82	CDL	PB2-OB3	5.86	1.71	1.50
12	D	242	CDL	PB2-OB3	5.68	1.70	1.50
12	A	447	CDL	PB2-OB3	5.58	1.70	1.50
13	A	448	PEE	P-O1P	5.55	1.70	1.50
12	A	447	CDL	PA1-OA3	5.37	1.69	1.50
13	E	197	PEE	P-O1P	5.25	1.69	1.50
12	G	82	CDL	PA1-OA3	5.23	1.68	1.50
12	D	242	CDL	PA1-OA3	5.16	1.68	1.50
13	C	380	PEE	P-O1P	5.10	1.68	1.50
12	G	82	CDL	OA8-CA7	5.05	1.48	1.33
12	D	242	CDL	OA6-CA5	5.02	1.48	1.34
12	G	82	CDL	OA6-CA5	4.95	1.48	1.34
12	G	82	CDL	OB6-CB5	4.92	1.48	1.34
12	D	242	CDL	OA8-CA7	4.86	1.47	1.33
12	A	447	CDL	OA6-CA5	4.70	1.47	1.34
13	A	448	PEE	O3-C30	4.53	1.46	1.33
13	C	380	PEE	O2-C10	4.53	1.47	1.34
12	A	447	CDL	OA8-CA7	4.38	1.46	1.33
14	C	381	HEC	CBD-CGD	-4.23	1.40	1.50
12	A	447	CDL	OB8-CB7	4.19	1.45	1.33
13	C	380	PEE	O3-C30	4.18	1.45	1.33
13	E	197	PEE	O3-C30	4.15	1.45	1.33
12	D	242	CDL	OB6-CB5	4.15	1.46	1.34
13	A	448	PEE	O2-C10	4.14	1.46	1.34
13	E	197	PEE	O2-C10	4.13	1.46	1.34
13	E	197	PEE	C18-C19	4.07	1.54	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	242	CDL	OB8-CB7	4.06	1.45	1.33
13	A	448	PEE	C18-C19	4.05	1.54	1.31
14	D	243	HEC	CBA-CGA	-4.00	1.41	1.50
13	C	380	PEE	C39-C38	3.99	1.54	1.31
13	A	448	PEE	C39-C38	3.97	1.54	1.31
13	C	380	PEE	C18-C19	3.84	1.53	1.31
13	E	197	PEE	C39-C38	3.79	1.53	1.31
12	A	447	CDL	OB6-CB5	3.77	1.44	1.34
12	G	82	CDL	OB8-CB7	3.67	1.44	1.33
14	C	382	HEC	CBA-CGA	-3.65	1.42	1.50
14	C	382	HEC	CBD-CGD	-3.61	1.42	1.50
14	D	243	HEC	CBD-CGD	-3.48	1.42	1.50
12	A	447	CDL	PA1-OA4	3.46	1.71	1.55
12	G	82	CDL	PA1-OA4	3.43	1.71	1.55
12	G	82	CDL	PB2-OB4	3.31	1.70	1.55
15	C	383	MYX	C2-C3	3.26	1.39	1.33
12	D	242	CDL	PB2-OB4	3.20	1.70	1.55
12	D	242	CDL	PA1-OA4	3.20	1.70	1.55
13	E	197	PEE	P-O2P	3.13	1.69	1.55
14	C	381	HEC	CBA-CGA	-3.12	1.43	1.50
13	A	448	PEE	P-O2P	3.00	1.69	1.55
12	A	447	CDL	PB2-OB4	2.94	1.68	1.55
14	C	382	HEC	FE-NA	2.89	2.04	1.95
14	D	243	HEC	CHD-C4C	2.89	1.45	1.39
14	C	382	HEC	FE-NB	2.80	2.03	1.94
17	J	63	PLX	O8-C24	2.79	1.45	1.40
13	C	380	PEE	P-O2P	2.79	1.68	1.55
14	C	382	HEC	CHD-C4C	2.73	1.45	1.39
15	C	383	MYX	C21-C20	2.64	1.52	1.44
14	D	243	HEC	FE-NB	2.61	2.02	1.94
14	D	243	HEC	FE-NA	2.47	2.03	1.95
14	D	243	HEC	FE-ND	2.38	2.02	1.94
14	C	381	HEC	CHD-C4C	2.27	1.44	1.39
17	J	63	PLX	C7-C6	2.26	1.55	1.50
14	C	382	HEC	FE-ND	2.24	2.01	1.94
14	C	382	HEC	FE-NC	2.20	2.02	1.95
14	C	381	HEC	FE-NA	2.10	2.02	1.95
12	D	242	CDL	C11-CA5	2.10	1.56	1.50
14	D	243	HEC	C4B-C3B	2.08	1.48	1.45
14	C	381	HEC	FE-NB	2.07	2.01	1.94

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	447	CDL	OB6-CB5-OB7	-6.87	107.64	123.70
12	G	82	CDL	OB8-CB7-OB9	-6.55	107.25	123.63
12	G	82	CDL	OA6-CA5-OA7	-6.10	109.44	123.70
12	D	242	CDL	OB6-CB5-OB7	-6.03	109.60	123.70
14	D	243	HEC	CHA-C1A-NA	6.03	131.02	124.45
14	D	243	HEC	CHB-C4A-NA	6.00	130.98	124.45
12	D	242	CDL	OB8-CB7-OB9	-5.77	109.20	123.63
14	C	382	HEC	CHB-C4A-NA	5.70	130.66	124.45
12	A	447	CDL	OA8-CA7-OA9	-5.54	109.76	123.63
13	A	448	PEE	O2-C10-O4	-5.52	110.80	123.70
14	C	381	HEC	C2A-C1A-NA	-5.48	105.03	110.32
12	A	447	CDL	OB8-CB7-OB9	-5.38	110.17	123.63
13	C	380	PEE	O3-C30-O5	-5.32	110.32	123.63
13	E	197	PEE	O2-C10-O4	-5.25	111.43	123.70
13	E	197	PEE	O3-C30-O5	-5.24	110.52	123.63
13	A	448	PEE	O3-C30-O5	-5.14	110.78	123.63
14	C	381	HEC	CHB-C4A-NA	4.74	129.61	124.45
15	C	383	MYX	C4-O2-C3	4.73	124.33	116.53
12	G	82	CDL	OA7-CA5-C11	-4.65	105.58	123.78
14	C	382	HEC	CHA-C1A-NA	4.51	129.37	124.45
14	C	381	HEC	CHA-C1A-NA	4.40	129.24	124.45
12	G	82	CDL	OB6-CB5-OB7	-4.38	113.45	123.70
14	D	243	HEC	C2A-C1A-NA	-4.28	106.20	110.32
12	D	242	CDL	OB7-CB5-C51	-4.20	107.36	123.78
14	C	381	HEC	C4A-CHB-C1B	-4.18	117.14	126.02
12	D	242	CDL	OA8-CA7-OA9	-4.12	113.33	123.63
14	C	381	HEC	C4C-CHD-C1D	-4.08	116.66	126.25
13	A	448	PEE	O4-C10-C11	-4.00	108.12	123.78
14	D	243	HEC	C4A-NA-C1A	4.00	112.34	105.82
12	G	82	CDL	OA8-CA7-OA9	-3.98	113.67	123.63
14	C	382	HEC	C4A-NA-C1A	3.96	112.28	105.82
12	G	82	CDL	OB9-CB7-C71	-3.96	108.29	123.78
14	C	382	HEC	C2A-C1A-NA	-3.96	106.50	110.32
13	C	380	PEE	O4-C10-C11	-3.95	108.34	123.78
14	C	381	HEC	C4A-NA-C1A	3.87	112.14	105.82
12	D	242	CDL	OA9-CA7-C31	-3.86	108.70	123.78
12	A	447	CDL	OA9-CA7-C31	-3.79	108.95	123.78
13	E	197	PEE	O4-C10-C11	-3.75	109.13	123.78
14	C	382	HEC	C1C-CHC-C4B	-3.72	117.50	126.25
12	D	242	CDL	OA6-CA5-OA7	-3.70	115.05	123.70
14	D	243	HEC	CHB-C1B-NB	3.64	128.34	124.42
15	C	383	MYX	C17-C19-C20	-3.60	118.33	125.83
13	A	448	PEE	O5-C30-C31	-3.59	109.72	123.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	447	CDL	OB9-CB7-C71	-3.58	109.78	123.78
12	G	82	CDL	OB7-CB5-C51	-3.53	109.97	123.78
12	D	242	CDL	OB9-CB7-C71	-3.52	110.01	123.78
15	C	383	MYX	C12-S1-C13	3.50	91.98	89.21
15	C	383	MYX	S1-C13-N2	-3.42	110.14	114.49
12	A	447	CDL	OB7-CB5-C51	-3.40	110.49	123.78
15	C	383	MYX	O3-C7-C5	3.39	114.71	107.73
14	C	382	HEC	CHB-C1B-NB	3.37	128.05	124.42
12	G	82	CDL	OA9-CA7-C31	-3.35	110.66	123.78
14	C	382	HEC	CHD-C1D-ND	3.32	128.48	124.37
14	C	382	HEC	C4A-CHB-C1B	-3.20	119.21	126.02
14	C	381	HEC	CHD-C1D-ND	3.20	128.32	124.37
14	D	243	HEC	C1A-CHA-C4D	-3.19	119.23	126.02
14	D	243	HEC	C4A-CHB-C1B	-3.17	119.29	126.02
13	E	197	PEE	O5-C30-C31	-3.16	111.44	123.78
14	C	382	HEC	C4C-CHD-C1D	-3.13	118.88	126.25
14	D	243	HEC	CHD-C1D-ND	3.04	128.13	124.37
14	C	382	HEC	C1A-CHA-C4D	-3.03	119.58	126.02
13	C	380	PEE	O2-C10-O4	-3.02	116.64	123.70
12	A	447	CDL	OA7-CA5-C11	-3.02	111.98	123.78
14	D	243	HEC	C1C-CHC-C4B	-2.91	119.41	126.25
13	C	380	PEE	O2-C2-C1	2.90	118.75	108.34
14	C	381	HEC	C1C-CHC-C4B	-2.86	119.52	126.25
12	A	447	CDL	OA6-CA5-OA7	-2.86	117.02	123.70
13	C	380	PEE	O5-C30-C31	-2.83	112.70	123.78
14	C	381	HEC	C1A-CHA-C4D	-2.82	120.02	126.02
15	C	383	MYX	C23-C22-C21	-2.82	120.29	126.13
14	C	381	HEC	CHC-C1C-NC	2.77	128.89	123.86
14	C	381	HEC	O2A-CGA-CBA	2.62	122.28	114.00
13	C	380	PEE	C2-O2-C10	2.55	123.91	117.80
14	D	243	HEC	C4C-CHD-C1D	-2.54	120.27	126.25
14	C	381	HEC	O2D-CGD-CBD	2.51	121.92	114.00
14	C	381	HEC	C1D-ND-C4D	2.50	108.17	105.21
14	C	382	HEC	C3A-C4A-NA	-2.49	105.03	109.64
14	C	382	HEC	O2D-CGD-CBD	2.43	121.67	114.00
14	D	243	HEC	C3A-C4A-NA	-2.43	105.14	109.64
13	A	448	PEE	O3-C3-C2	2.40	115.33	108.40
14	C	381	HEC	CAC-C3C-C4C	2.37	128.18	124.91
14	D	243	HEC	CHA-C4D-ND	2.32	126.92	124.42
14	C	381	HEC	C3A-C4A-NA	-2.29	105.40	109.64
12	G	82	CDL	OA6-CA4-CA3	2.25	116.43	108.34
14	C	381	HEC	C3C-C4C-NC	-2.22	107.68	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	383	MYX	C10-C11-C12	-2.22	118.78	126.39
14	D	243	HEC	CAA-CBA-CGA	-2.18	107.89	113.67
12	G	82	CDL	OA6-CA5-C11	2.17	116.18	111.48
14	C	381	HEC	CAC-C3C-C2C	-2.17	123.46	126.89
14	D	243	HEC	CHB-C1B-C2B	-2.12	121.69	125.03
14	C	381	HEC	C3D-C4D-ND	-2.11	108.31	110.35
15	C	383	MYX	C12-C11-N2	2.10	117.06	113.56
14	D	243	HEC	CHD-C4C-NC	2.09	127.66	123.86
14	C	382	HEC	CHD-C4C-NC	2.08	127.64	123.86
14	C	381	HEC	CHB-C1B-NB	2.05	126.63	124.42
15	C	383	MYX	S2-C16-N3	-2.01	111.56	114.19
14	D	243	HEC	CHC-C1C-NC	2.01	127.51	123.86
14	C	381	HEC	CAA-C2A-C3A	-2.01	124.11	127.87

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	A	447	CDL	CA4
12	D	242	CDL	CA4
12	G	82	CDL	CA4
14	C	382	HEC	NA
14	D	243	HEC	NA

All (253) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	447	CDL	CA3-OA5-PA1-OA2
12	A	447	CDL	CA3-OA5-PA1-OA3
12	A	447	CDL	CA3-OA5-PA1-OA4
12	A	447	CDL	CB3-OB5-PB2-OB2
12	A	447	CDL	CB3-OB5-PB2-OB3
12	A	447	CDL	OB6-CB4-CB6-OB8
12	A	447	CDL	OB7-CB5-OB6-CB4
12	D	242	CDL	O1-C1-CA2-OA2
12	D	242	CDL	CA2-OA2-PA1-OA4
12	D	242	CDL	CA2-OA2-PA1-OA5
12	D	242	CDL	CA3-OA5-PA1-OA4
12	D	242	CDL	C11-CA5-OA6-CA4
12	D	242	CDL	CB2-OB2-PB2-OB4
12	D	242	CDL	CB2-OB2-PB2-OB5
12	D	242	CDL	OB7-CB5-OB6-CB4
12	G	82	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
12	G	82	CDL	CA2-OA2-PA1-OA5
12	G	82	CDL	CA3-OA5-PA1-OA2
12	G	82	CDL	CA3-OA5-PA1-OA3
12	G	82	CDL	CB3-OB5-PB2-OB2
12	G	82	CDL	CB3-OB5-PB2-OB3
12	G	82	CDL	CB3-OB5-PB2-OB4
12	G	82	CDL	OB9-CB7-OB8-CB6
13	A	448	PEE	C1-O3P-P-O2P
13	A	448	PEE	C4-O4P-P-O3P
13	A	448	PEE	C4-O4P-P-O1P
13	A	448	PEE	O4P-C4-C5-N
17	J	63	PLX	O7-C6-O6-C4
17	J	63	PLX	C3-O4-P1-O1
17	J	63	PLX	C3-O4-P1-O3
17	J	63	PLX	C25-C24-O8-C5
12	D	242	CDL	OB9-CB7-OB8-CB6
14	D	243	HEC	C2B-C3B-CAB-CBB
12	A	447	CDL	OB9-CB7-OB8-CB6
12	D	242	CDL	OA7-CA5-OA6-CA4
12	G	82	CDL	OA7-CA5-OA6-CA4
13	E	197	PEE	O4-C10-O2-C2
12	D	242	CDL	C71-CB7-OB8-CB6
12	G	82	CDL	C31-CA7-OA8-CA6
13	A	448	PEE	C17-C18-C19-C20
12	A	447	CDL	OA9-CA7-OA8-CA6
13	A	448	PEE	O4-C10-O2-C2
12	A	447	CDL	O1-C1-CB2-OB2
12	D	242	CDL	O1-C1-CB2-OB2
12	G	82	CDL	O1-C1-CB2-OB2
13	A	448	PEE	O5-C30-O3-C3
12	A	447	CDL	C11-CA5-OA6-CA4
13	C	380	PEE	C11-C10-O2-C2
13	C	380	PEE	O5-C30-O3-C3
14	D	243	HEC	C2A-CAA-CBA-CGA
13	E	197	PEE	O5-C30-O3-C3
12	G	82	CDL	C71-CB7-OB8-CB6
13	A	448	PEE	C37-C38-C39-C40
13	C	380	PEE	C17-C18-C19-C20
13	C	380	PEE	C37-C38-C39-C40
12	D	242	CDL	CA2-C1-CB2-OB2
12	A	447	CDL	C71-CB7-OB8-CB6
13	C	380	PEE	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
12	A	447	CDL	O1-C1-CA2-OA2
14	D	243	HEC	C4B-C3B-CAB-CBB
12	D	242	CDL	CA7-C31-C32-C33
12	A	447	CDL	CB5-C51-C52-C53
13	C	380	PEE	C10-C11-C12-C13
13	E	197	PEE	C10-C11-C12-C13
12	A	447	CDL	CA2-C1-CB2-OB2
12	D	242	CDL	CB2-C1-CA2-OA2
12	G	82	CDL	CA2-C1-CB2-OB2
17	J	63	PLX	O6-C6-C7-C8
12	A	447	CDL	C51-CB5-OB6-CB4
12	D	242	CDL	C31-C32-C33-C34
17	J	63	PLX	C30-C31-C32-C33
13	C	380	PEE	C22-C23-C24-C25
12	G	82	CDL	OA9-CA7-OA8-CA6
12	A	447	CDL	C14-C15-C16-C17
12	G	82	CDL	C31-C32-C33-C34
13	C	380	PEE	C20-C21-C22-C23
17	J	63	PLX	C14-C15-C16-C17
17	J	63	PLX	C11-C10-C9-C8
12	D	242	CDL	C51-C52-C53-C54
13	C	380	PEE	C31-C32-C33-C34
12	D	242	CDL	C51-CB5-OB6-CB4
12	A	447	CDL	C72-C73-C74-C75
12	A	447	CDL	C34-C35-C36-C37
12	D	242	CDL	C54-C55-C56-C57
12	G	82	CDL	CB3-CB4-CB6-OB8
12	G	82	CDL	C12-C13-C14-C15
12	G	82	CDL	C74-C75-C76-C77
12	A	447	CDL	C53-C54-C55-C56
12	D	242	CDL	C13-C14-C15-C16
13	E	197	PEE	C31-C32-C33-C34
13	E	197	PEE	C34-C35-C36-C37
12	D	242	CDL	OA9-CA7-OA8-CA6
13	A	448	PEE	C40-C41-C42-C43
17	J	63	PLX	C35-C36-C37-C38
13	A	448	PEE	C10-C11-C12-C13
17	J	63	PLX	C33-C34-C35-C36
17	J	63	PLX	C34-C35-C36-C37
12	G	82	CDL	OB7-CB5-OB6-CB4
12	D	242	CDL	C34-C35-C36-C37
17	J	63	PLX	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
13	A	448	PEE	C22-C23-C24-C25
12	G	82	CDL	C14-C15-C16-C17
13	E	197	PEE	C22-C23-C24-C25
12	G	82	CDL	C11-CA5-OA6-CA4
12	A	447	CDL	C13-C14-C15-C16
13	A	448	PEE	C15-C16-C17-C18
13	C	380	PEE	C19-C20-C21-C22
13	C	380	PEE	C15-C16-C17-C18
13	A	448	PEE	C21-C22-C23-C24
17	J	63	PLX	C31-C32-C33-C34
17	J	63	PLX	C27-C28-C29-C30
12	A	447	CDL	C54-C55-C56-C57
17	J	63	PLX	C16-C17-C18-C19
12	D	242	CDL	C33-C34-C35-C36
12	A	447	CDL	C32-C33-C34-C35
12	D	242	CDL	C73-C74-C75-C76
12	G	82	CDL	C73-C74-C75-C76
13	C	380	PEE	C11-C12-C13-C14
13	E	197	PEE	C32-C33-C34-C35
17	J	63	PLX	C12-C13-C14-C15
12	G	82	CDL	C53-C54-C55-C56
17	J	63	PLX	C9-C10-C11-C12
13	C	380	PEE	C39-C40-C41-C42
13	E	197	PEE	C41-C42-C43-C44
12	G	82	CDL	C32-C33-C34-C35
12	A	447	CDL	C51-C52-C53-C54
12	G	82	CDL	CA3-CA4-CA6-OA8
13	E	197	PEE	C35-C36-C37-C38
12	G	82	CDL	C11-C12-C13-C14
13	A	448	PEE	C12-C13-C14-C15
13	E	197	PEE	C13-C14-C15-C16
13	E	197	PEE	C21-C22-C23-C24
13	A	448	PEE	C39-C40-C41-C42
13	E	197	PEE	C15-C16-C17-C18
12	G	82	CDL	C15-C16-C17-C18
13	E	197	PEE	C42-C43-C44-C45
12	G	82	CDL	C35-C36-C37-C38
13	A	448	PEE	C20-C21-C22-C23
12	A	447	CDL	C75-C76-C77-C78
12	A	447	CDL	C74-C75-C76-C77
13	A	448	PEE	C24-C25-C26-C27
17	J	63	PLX	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
12	A	447	CDL	OB5-CB3-CB4-CB6
12	G	82	CDL	OA5-CA3-CA4-CA6
12	D	242	CDL	C55-C56-C57-C58
13	E	197	PEE	C24-C25-C26-C27
12	D	242	CDL	C71-C72-C73-C74
12	A	447	CDL	CB3-CB4-CB6-OB8
17	J	63	PLX	C20-C21-C22-C23
12	A	447	CDL	C52-C53-C54-C55
13	A	448	PEE	C42-C43-C44-C45
12	A	447	CDL	C1-CA2-OA2-PA1
14	C	382	HEC	C4B-C3B-CAB-CBB
13	A	448	PEE	C35-C36-C37-C38
17	J	63	PLX	C19-C20-C21-C22
17	J	63	PLX	C13-C14-C15-C16
13	E	197	PEE	C37-C38-C39-C40
13	C	380	PEE	C41-C42-C43-C44
12	A	447	CDL	OB5-CB3-CB4-OB6
12	D	242	CDL	CB5-C51-C52-C53
12	D	242	CDL	C11-C12-C13-C14
12	D	242	CDL	OB6-CB4-CB6-OB8
12	G	82	CDL	OB6-CB4-CB6-OB8
17	J	63	PLX	C25-C26-C27-C28
13	C	380	PEE	C32-C33-C34-C35
12	G	82	CDL	CB5-C51-C52-C53
17	J	63	PLX	C29-C30-C31-C32
13	A	448	PEE	C30-C31-C32-C33
13	E	197	PEE	C11-C12-C13-C14
17	J	63	PLX	C32-C33-C34-C35
13	C	380	PEE	C13-C14-C15-C16
12	D	242	CDL	OA5-CA3-CA4-OA6
12	G	82	CDL	OA5-CA3-CA4-OA6
12	G	82	CDL	C52-C53-C54-C55
12	A	447	CDL	CA2-OA2-PA1-OA5
12	A	447	CDL	CB2-OB2-PB2-OB3
12	A	447	CDL	CB2-OB2-PB2-OB4
12	A	447	CDL	CB2-OB2-PB2-OB5
12	A	447	CDL	CB3-OB5-PB2-OB4
12	D	242	CDL	CA2-OA2-PA1-OA3
12	D	242	CDL	CA3-OA5-PA1-OA2
12	D	242	CDL	CA3-OA5-PA1-OA3
12	D	242	CDL	CB2-OB2-PB2-OB3
12	G	82	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
13	A	448	PEE	C1-O3P-P-O1P
13	A	448	PEE	C1-O3P-P-O4P
13	A	448	PEE	C4-O4P-P-O2P
13	C	380	PEE	C1-O3P-P-O1P
13	C	380	PEE	C1-O3P-P-O4P
13	E	197	PEE	C4-O4P-P-O1P
17	J	63	PLX	C3-O4-P1-O2
13	C	380	PEE	C40-C41-C42-C43
13	A	448	PEE	C31-C32-C33-C34
13	C	380	PEE	C14-C15-C16-C17
17	J	63	PLX	O7-C6-C7-C8
17	J	63	PLX	C10-C11-C12-C13
12	D	242	CDL	C1-CB2-OB2-PB2
17	J	63	PLX	C6-C7-C8-C9
13	A	448	PEE	C38-C39-C40-C41
12	G	82	CDL	C13-C14-C15-C16
17	J	63	PLX	C17-C18-C19-C20
14	C	382	HEC	CAA-CBA-CGA-O2A
12	G	82	CDL	CB2-C1-CA2-OA2
14	D	243	HEC	CAA-CBA-CGA-O1A
12	G	82	CDL	CA3-CA4-OA6-CA5
13	C	380	PEE	C1-C2-O2-C10
14	D	243	HEC	CAA-CBA-CGA-O2A
17	J	63	PLX	O4-C3-C4-O6
12	A	447	CDL	CB7-C71-C72-C73
14	C	381	HEC	CAA-CBA-CGA-O1A
14	C	382	HEC	CAA-CBA-CGA-O1A
12	D	242	CDL	CB7-C71-C72-C73
12	D	242	CDL	C14-C15-C16-C17
14	C	382	HEC	C4C-C3C-CAC-CBC
14	C	381	HEC	CAA-CBA-CGA-O2A
12	G	82	CDL	C1-CA2-OA2-PA1
12	G	82	CDL	C71-C72-C73-C74
14	C	382	HEC	C3D-CAD-CBD-CGD
14	C	381	HEC	CAD-CBD-CGD-O2D
13	E	197	PEE	C30-C31-C32-C33
14	D	243	HEC	CAD-CBD-CGD-O1D
13	A	448	PEE	C23-C24-C25-C26
17	J	63	PLX	C4-C5-O8-C24
14	C	382	HEC	C2B-C3B-CAB-CBB
12	G	82	CDL	O1-C1-CA2-OA2
12	A	447	CDL	CB2-C1-CA2-OA2

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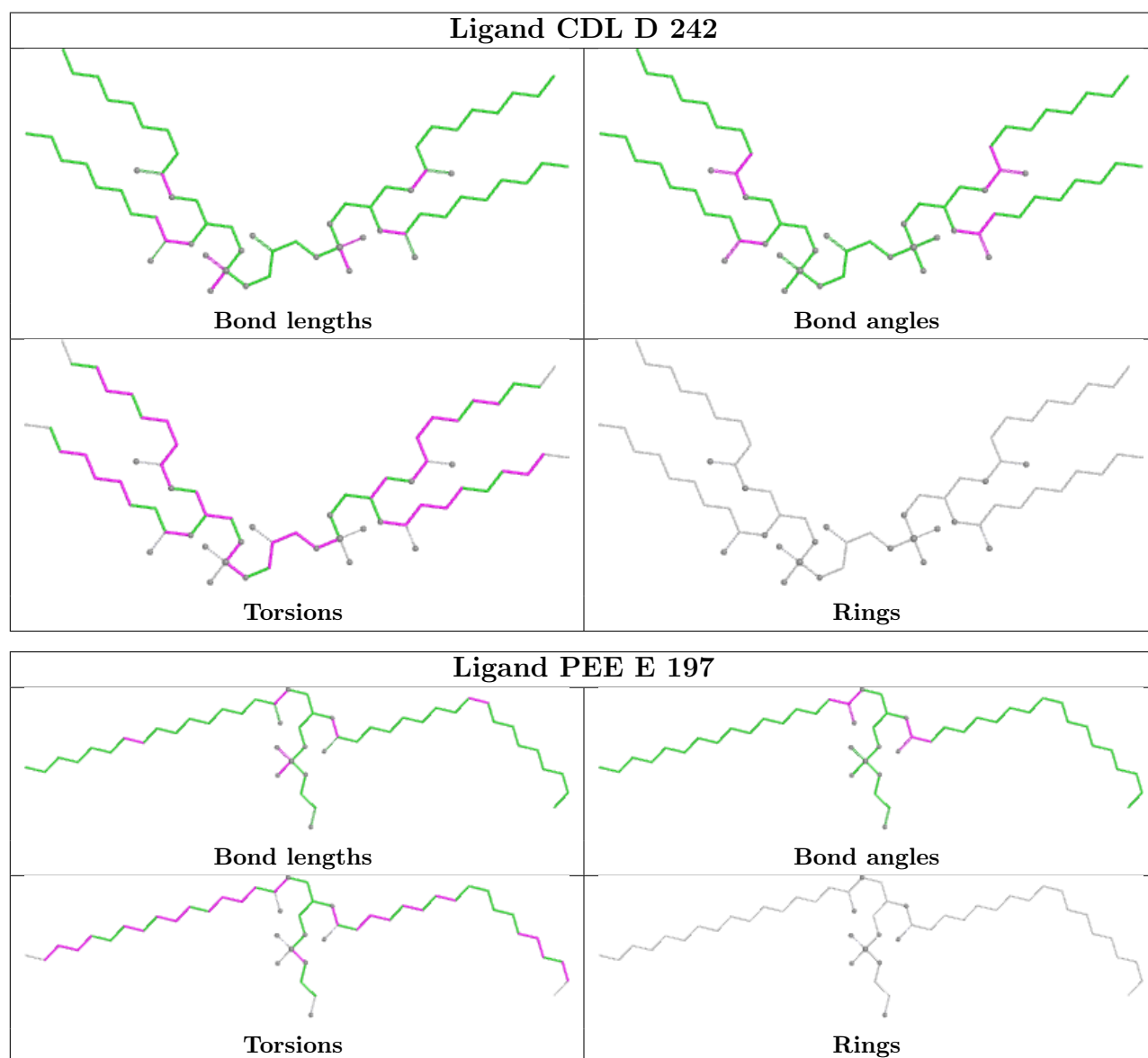
Mol	Chain	Res	Type	Atoms
14	D	243	HEC	CAD-CBD-CGD-O2D
12	D	242	CDL	CB3-CB4-CB6-OB8
12	G	82	CDL	C12-C11-CA5-OA6
12	D	242	CDL	OA5-CA3-CA4-CA6
13	A	448	PEE	O3P-C1-C2-C3
17	J	63	PLX	C7-C6-O6-C4
12	D	242	CDL	C12-C13-C14-C15
17	J	63	PLX	N1-C1-C2-O1
13	A	448	PEE	C11-C10-O2-C2
17	J	63	PLX	C11-C12-C13-C14
13	C	380	PEE	C42-C43-C44-C45
14	C	382	HEC	CAD-CBD-CGD-O1D
14	C	382	HEC	CAD-CBD-CGD-O2D
13	A	448	PEE	O2-C10-C11-C12
12	D	242	CDL	CA3-CA4-CA6-OA8
14	C	381	HEC	CAD-CBD-CGD-O1D
14	D	243	HEC	C2C-C3C-CAC-CBC
17	J	63	PLX	C2-C1-N1-C1C
12	D	242	CDL	C32-C31-CA7-OA9
12	D	242	CDL	C72-C71-CB7-OB9
12	G	82	CDL	C32-C31-CA7-OA9
13	C	380	PEE	O4-C10-C11-C12
17	J	63	PLX	O9-C24-O8-C5
12	D	242	CDL	C52-C51-CB5-OB7
12	A	447	CDL	C35-C36-C37-C38
13	E	197	PEE	C40-C41-C42-C43
13	C	380	PEE	C36-C37-C38-C39

There are no ring outliers.

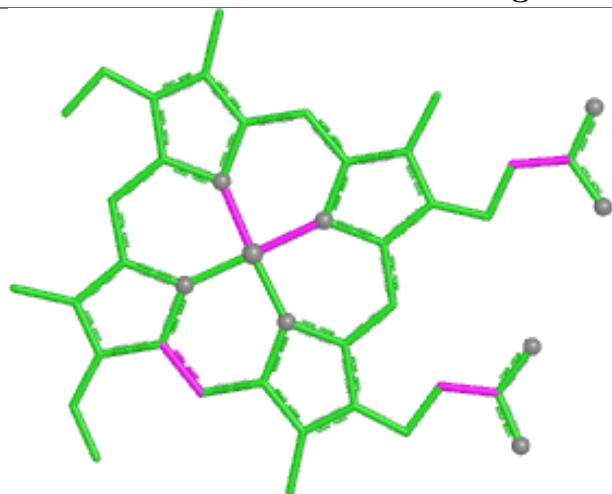
10 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	E	197	PEE	3	0
14	C	381	HEC	6	0
15	C	383	MYX	1	0
14	C	382	HEC	4	0
12	A	447	CDL	1	0
13	C	380	PEE	1	0
13	A	448	PEE	1	0
14	D	243	HEC	11	0
12	G	82	CDL	2	0
17	J	63	PLX	4	0

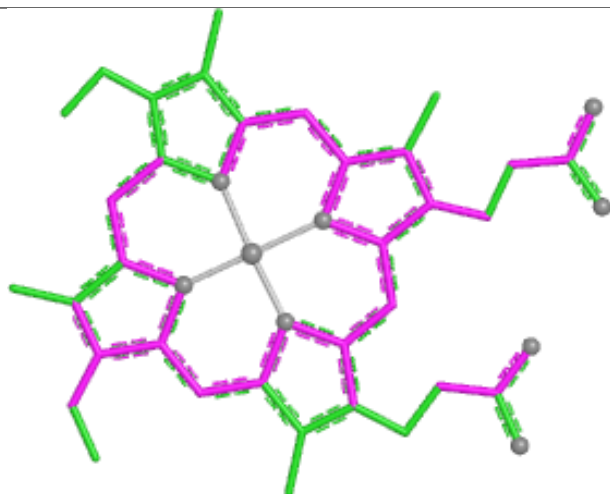
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



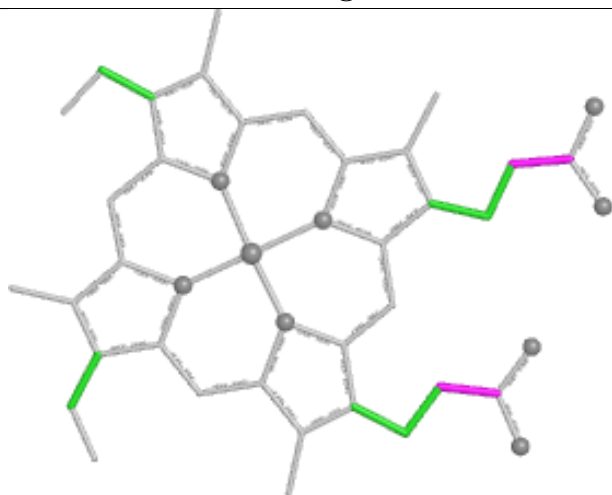
Ligand HEC C 381



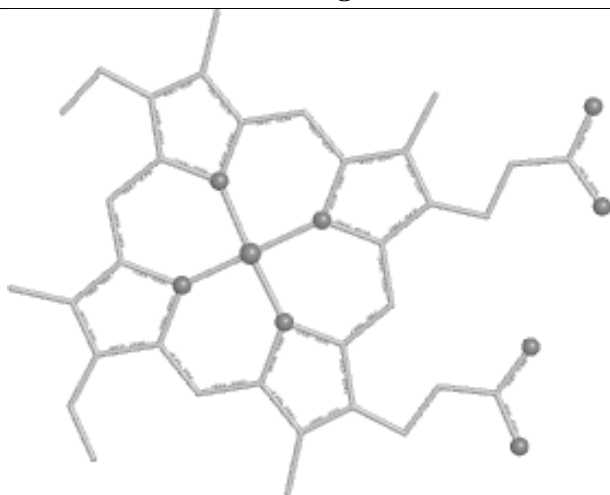
Bond lengths



Bond angles

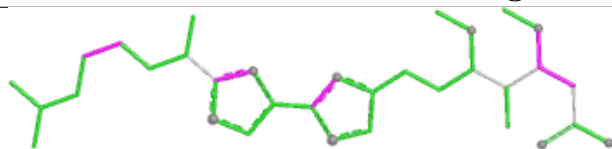


Torsions

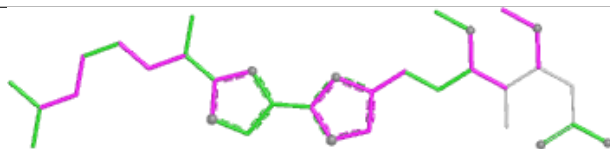


Rings

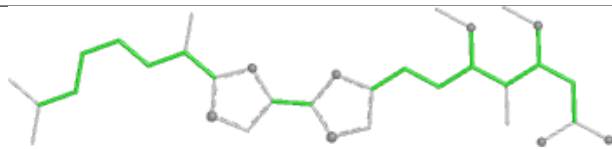
Ligand MYX C 383



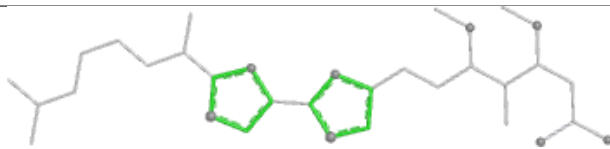
Bond lengths



Bond angles

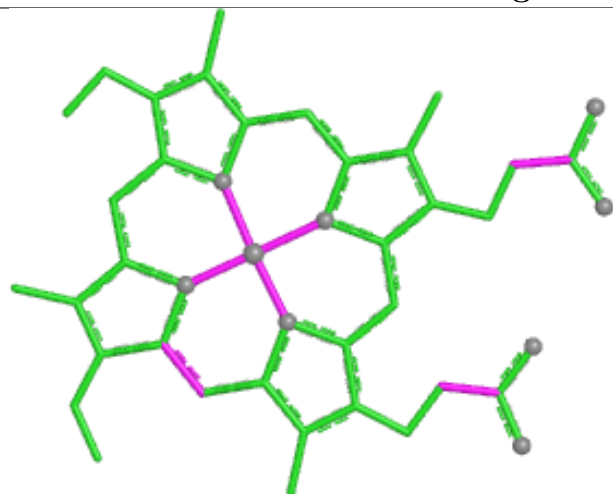


Torsions

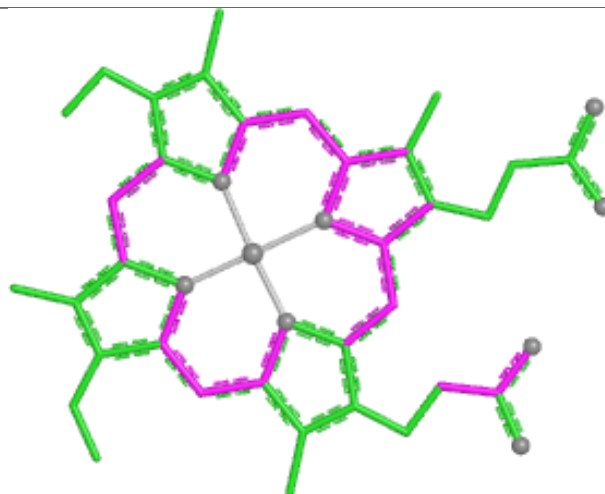


Rings

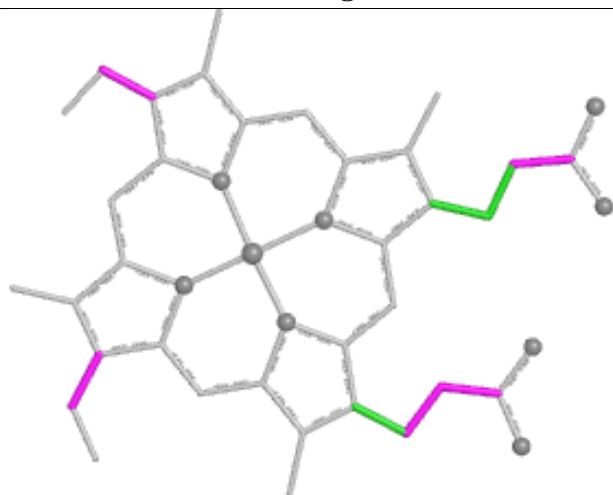
Ligand HEC C 382



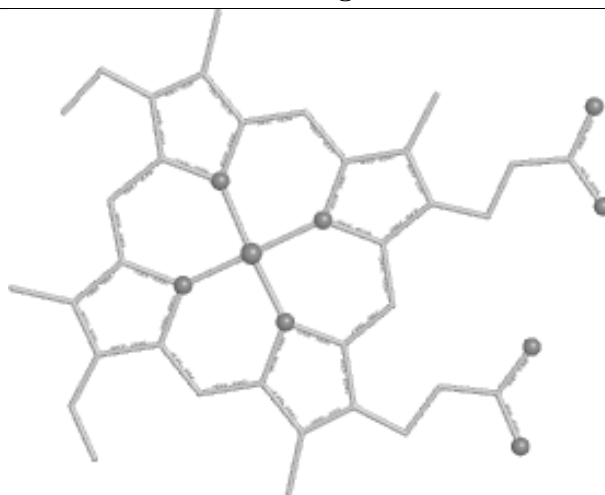
Bond lengths



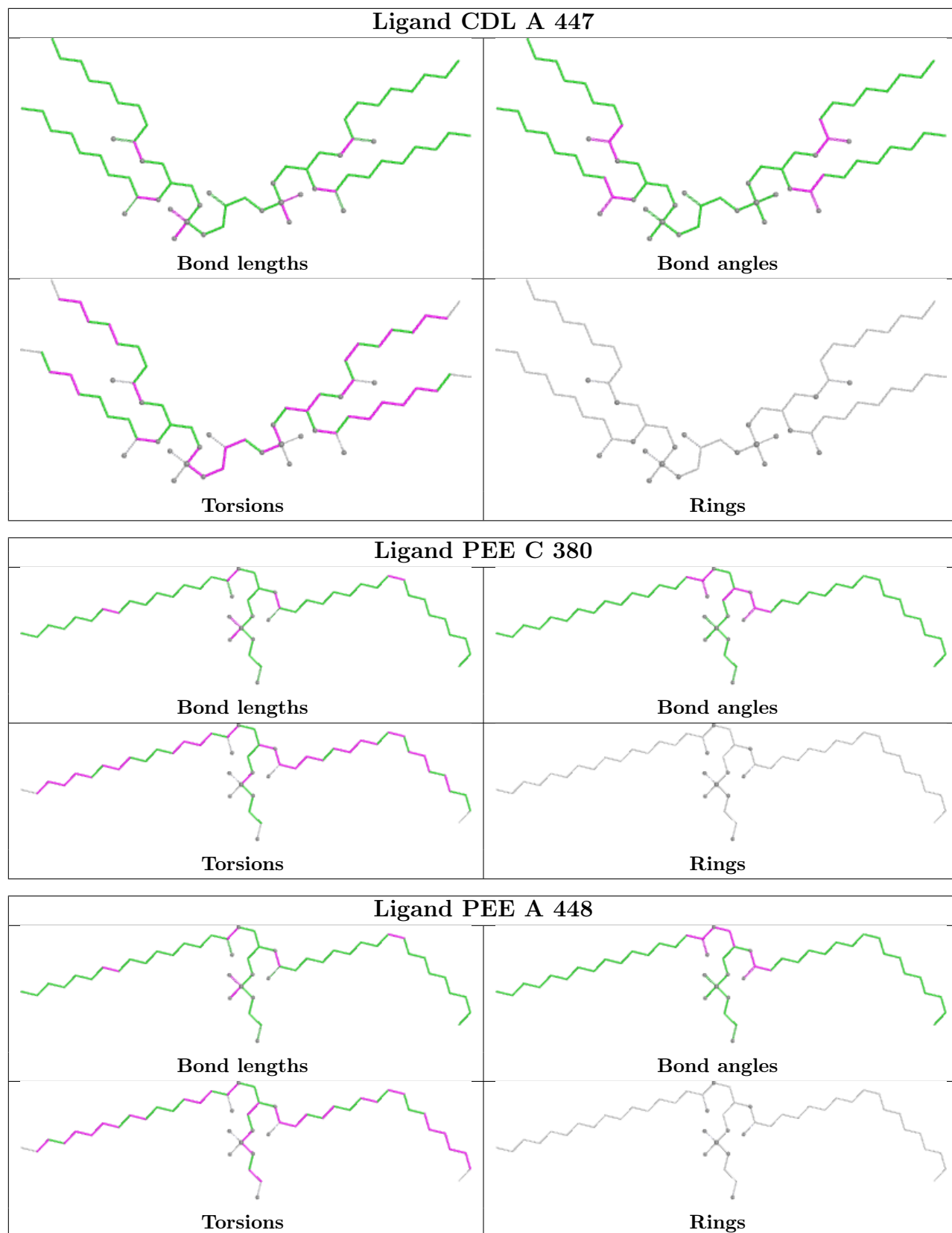
Bond angles

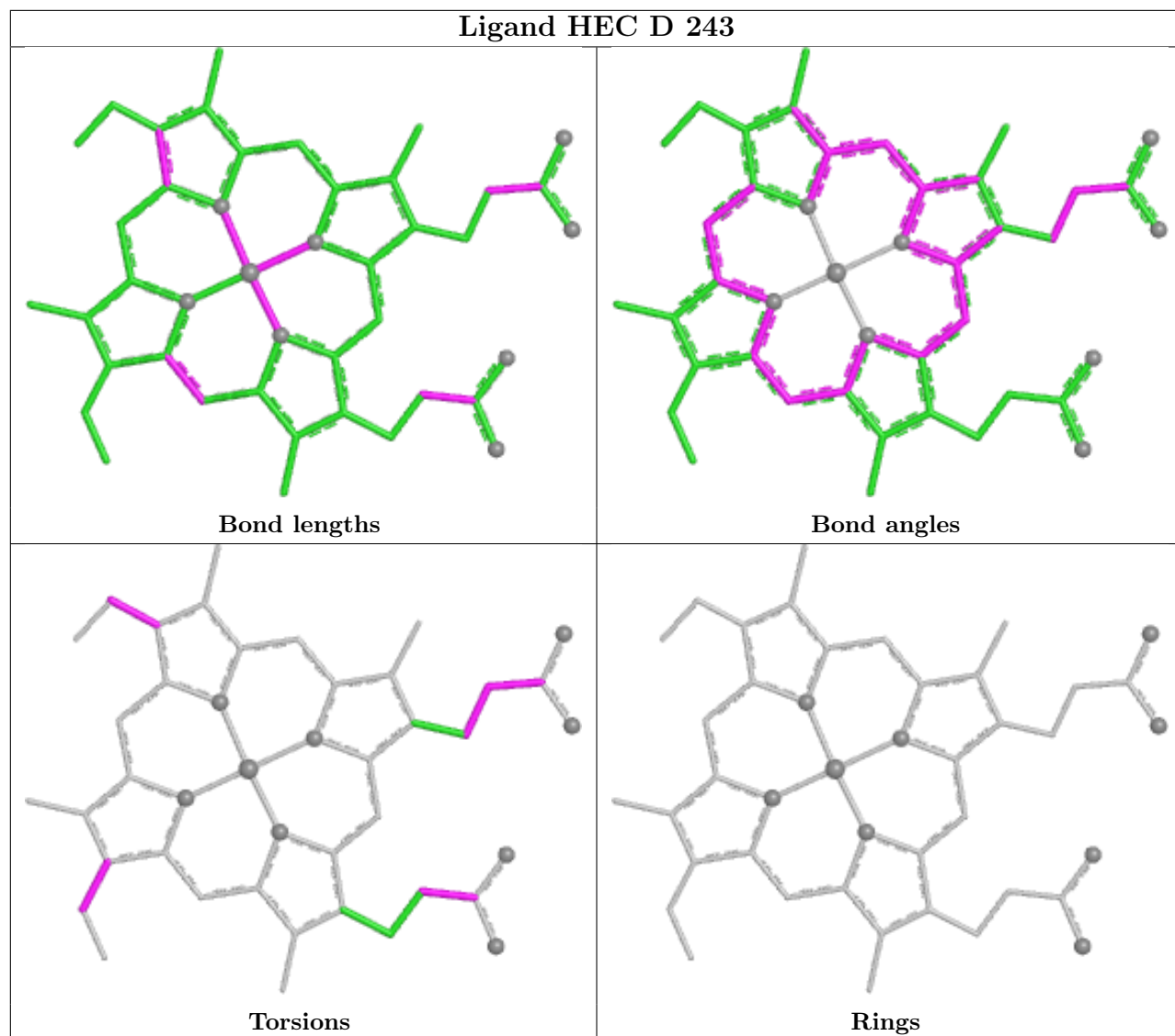


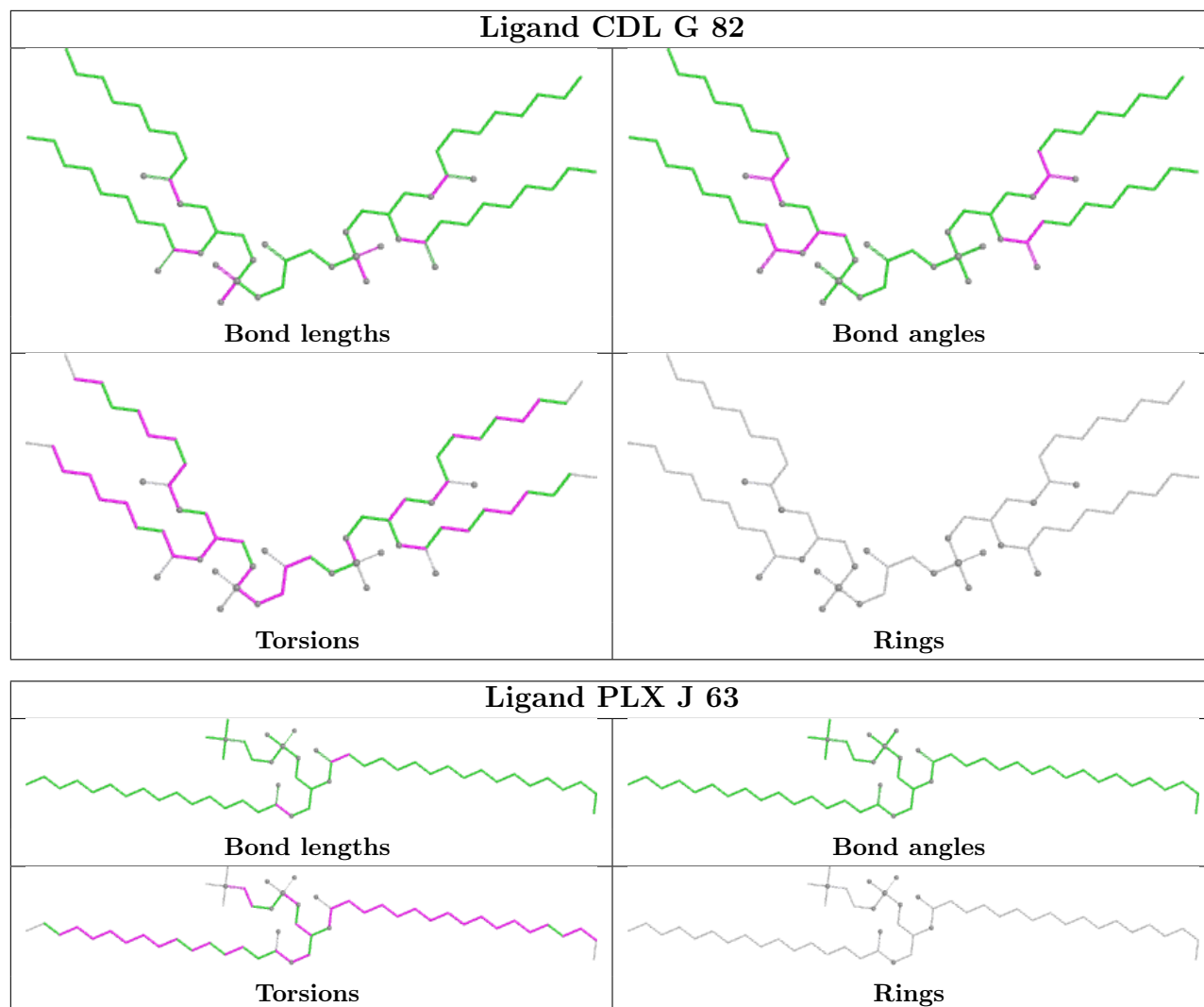
Torsions



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.