



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 09:00 AM EDT

PDB ID : 1SQX / pdb_00001sqx
Title : Crystal Structure Analysis of Bovine Bcl with Stigmatellin A
Authors : Esser, L.; Quinn, B.; Li, Y.F.; Zhang, M.; Elberry, M.; Yu, L.; Yu, C.A.; Xia, D.
Deposited on : 2004-03-21
Resolution : 2.60 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

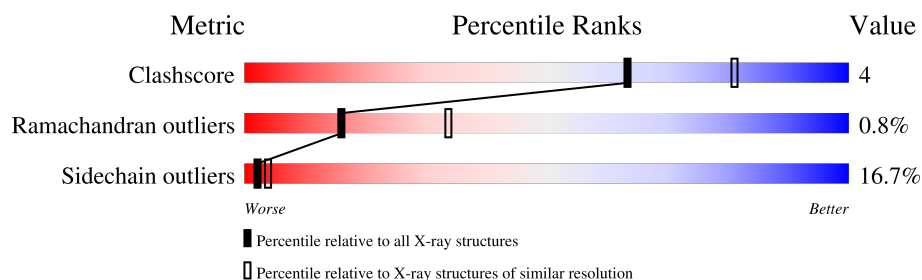
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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	81% 16% .
2	B	439	77% 15% . .
3	C	379	74% 22% . .
4	E	196	79% 20% .
5	D	241	74% 20% 5%
6	G	81	72% 16% 5% 7%
7	I	78	31% 29% 9% . 27%
8	F	110	76% 15% 5% 5%

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

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
13	HEC	C	382	X	-	-	-
13	HEC	D	242	X	-	-	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 16978 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	E	196	Total	C	N	O	S	0	0	0
			1519	957	263	291	8			

- 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	D	241	Total	C	N	O	S	0	0	0
			1919	1225	330	349	15			

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

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

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

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

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

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

- 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	K	53	Total	C	N	O	S	0	0	0
			438	293	78	66	1			

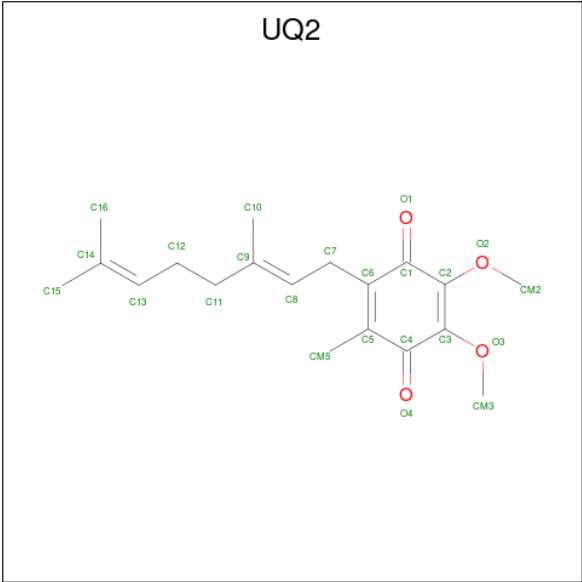
- Molecule 10 is a protein called Ubiquinol-cytochrome C reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	67	Total	C	N	O	S	0	0	0
			548	332	99	112	5			

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

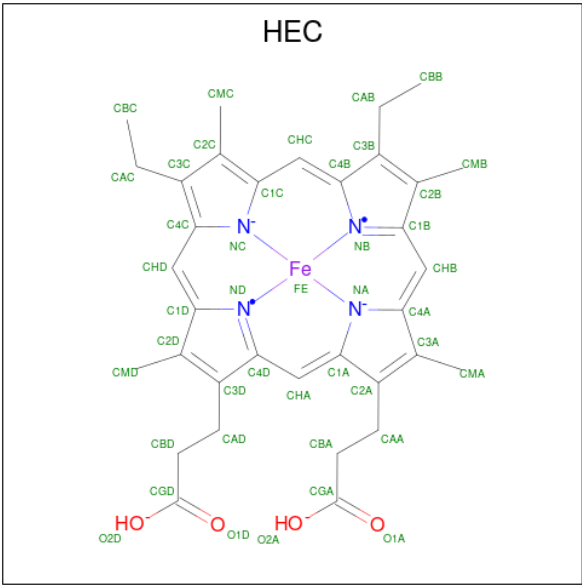
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	J	60	Total	C	N	O	0	0	0
			495	324	86	85			

- Molecule 12 is UBIQUINONE-2 (CCD ID: UQ2) (formula: C₁₉H₂₆O₄).



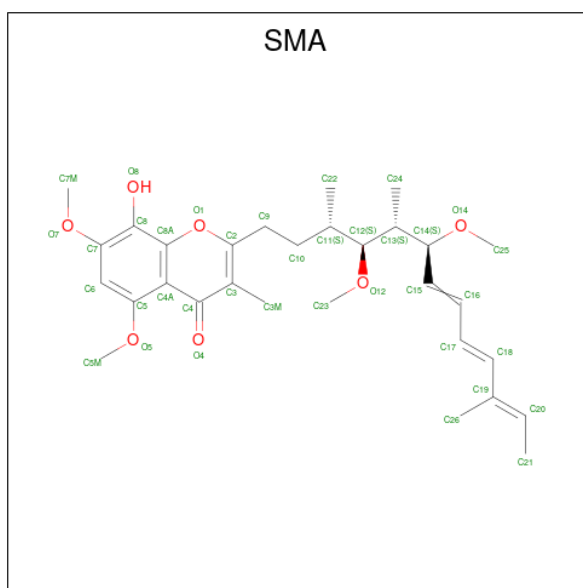
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	1	Total	C	O		0	0
			23	19	4			

- Molecule 13 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



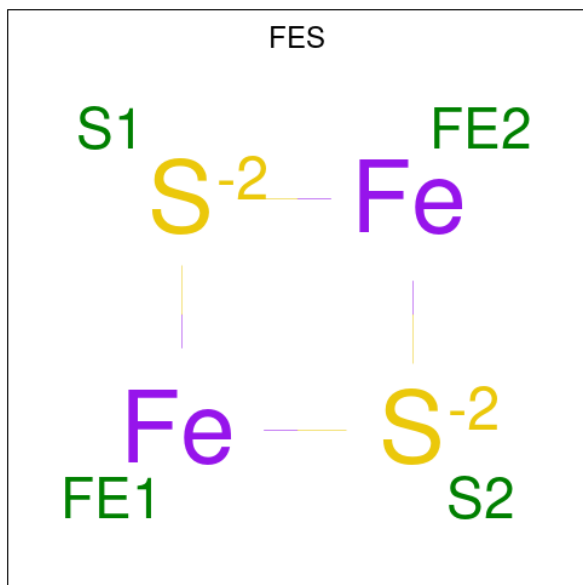
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
13	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
13	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 14 is STIGMATELLIN A (CCD ID: SMA) (formula: $C_{30}H_{42}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	C	O	0	0
			37	30	7		

- 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.

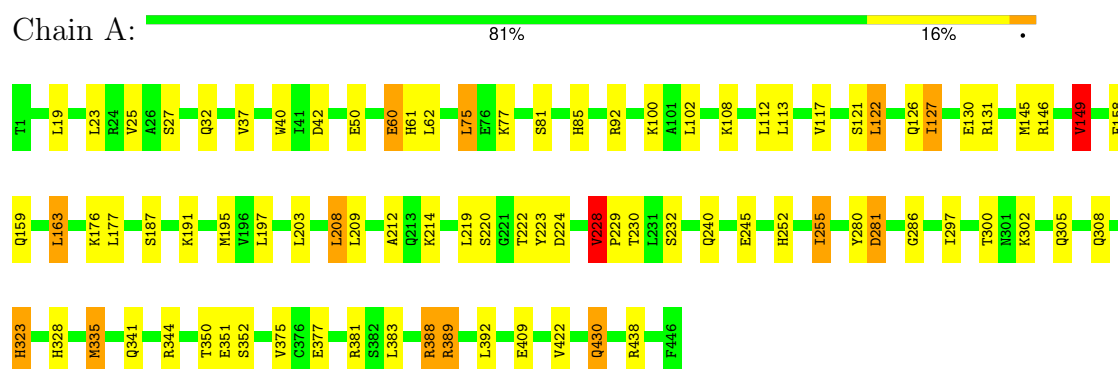
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	65	Total 65	O 65	0	0
16	B	99	Total 99	O 99	0	0
16	C	36	Total 36	O 36	0	0
16	E	8	Total 8	O 8	0	0
16	D	19	Total 19	O 19	0	0
16	G	19	Total 19	O 19	0	0
16	I	2	Total 2	O 2	0	0
16	F	32	Total 32	O 32	0	0
16	K	2	Total 2	O 2	0	0
16	H	6	Total 6	O 6	0	0

3 Residue-property plots

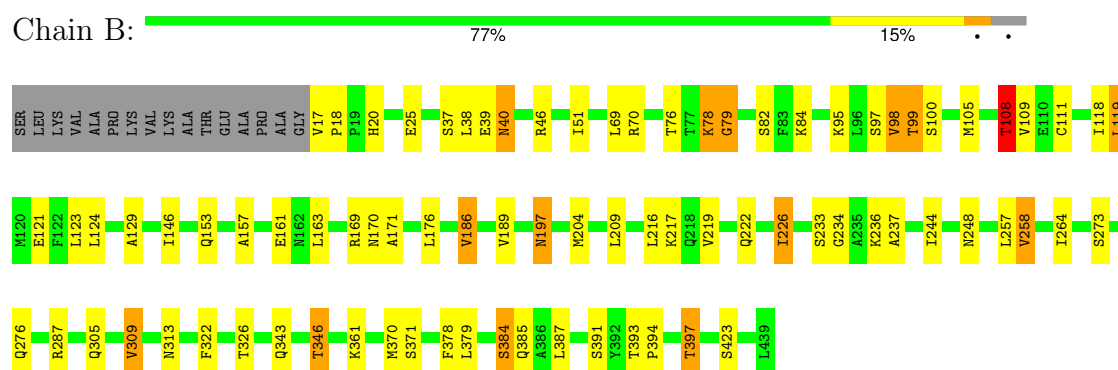
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

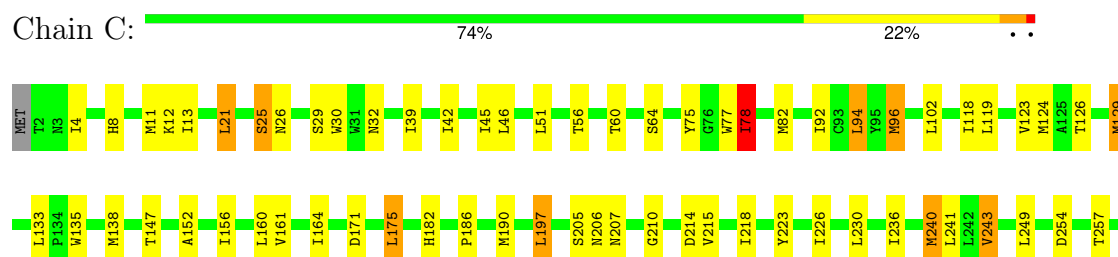
- Molecule 1: Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial precursor

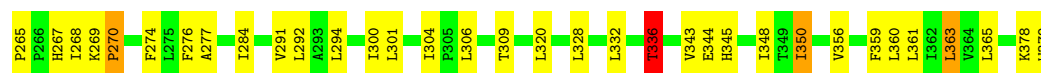


- Molecule 2: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial precursor



- Molecule 3: Cytochrome b





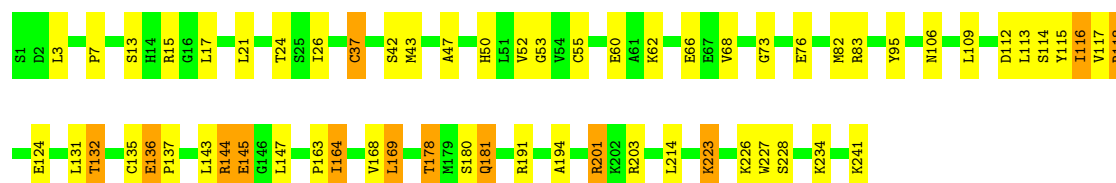
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain E: 79% 20%



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

Chain D: 74% 20% 5%



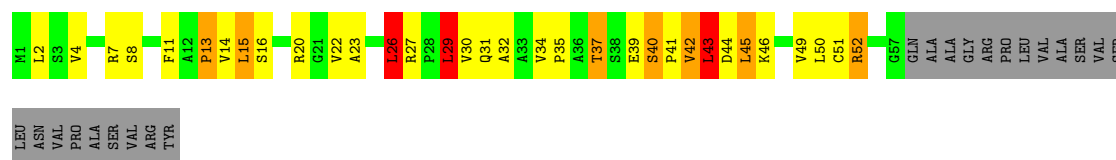
- Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein

Chain G: 72% 16% 5% 7%



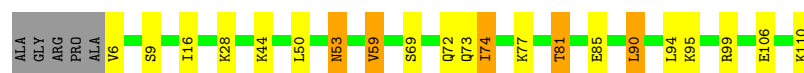
- Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C

Chain I: 31% 29% 9% 27%



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

Chain F: 76% 15% 5% 5%



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

Chain K:  62% 29% 5%



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

Chain H:  55% 31% 14%



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

Chain J:  76% 19% 5%



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	154.38Å 154.38Å 590.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60	Depositor
% Data completeness (in resolution range)	94.2 (40.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.233 , 0.281	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16978	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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: HEC, FES, SMA, 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	1.00	5/3531 (0.1%)	1.06	3/4792 (0.1%)
2	B	1.05	9/3232 (0.3%)	1.07	2/4386 (0.0%)
3	C	1.14	14/3100 (0.5%)	1.16	3/4242 (0.1%)
4	E	1.16	5/1553 (0.3%)	1.05	1/2100 (0.0%)
5	D	1.06	4/1978 (0.2%)	1.08	1/2684 (0.0%)
6	G	1.33	2/649 (0.3%)	1.14	1/878 (0.1%)
7	I	1.49	4/411 (1.0%)	1.18	1/558 (0.2%)
8	F	1.06	3/930 (0.3%)	1.09	0/1246
9	K	1.21	2/454 (0.4%)	1.16	0/621
10	H	1.07	2/553 (0.4%)	1.17	0/741
11	J	1.12	1/508 (0.2%)	1.19	0/686
All	All	1.10	51/16899 (0.3%)	1.10	12/22934 (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	4
2	B	0	7
3	C	0	2
4	E	0	1
5	D	0	5
7	I	0	8
11	J	0	1
All	All	0	28

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	34	ILE	CA-CB	15.12	1.61	1.54
2	B	105	MET	SD-CE	-9.58	1.55	1.79
1	A	127	ILE	CA-CB	8.79	1.66	1.54
8	F	59	VAL	CA-CB	8.50	1.65	1.54
2	B	146	ILE	CA-CB	7.14	1.62	1.54
3	C	39	ILE	CA-CB	6.81	1.61	1.54
1	A	228	VAL	CA-CB	6.71	1.60	1.53
5	D	137	PRO	CA-C	6.69	1.55	1.51
11	J	42	ILE	CA-CB	6.66	1.62	1.54
3	C	240	MET	SD-CE	-6.65	1.62	1.79
7	I	42	VAL	CA-CB	6.57	1.63	1.54
3	C	350	ILE	CA-CB	6.49	1.63	1.54
3	C	336	THR	CA-CB	6.45	1.64	1.53
7	I	49	VAL	CA-CB	6.44	1.61	1.54
6	G	37	VAL	CA-CB	6.42	1.62	1.54
2	B	189	VAL	CA-CB	6.37	1.61	1.54
5	D	7	PRO	CA-C	6.23	1.55	1.51
8	F	81	THR	CA-CB	6.15	1.60	1.53
4	E	171	ILE	CA-CB	6.09	1.61	1.54
3	C	92	ILE	CA-CB	6.07	1.61	1.54
10	H	14	VAL	CA-CB	5.91	1.60	1.53
2	B	244	ILE	CA-CB	5.91	1.61	1.54
9	K	48	ILE	CA-CB	5.86	1.62	1.54
2	B	394	PRO	CA-C	5.85	1.57	1.52
7	I	30	VAL	CA-CB	5.84	1.62	1.54
9	K	18	VAL	CA-CB	5.82	1.61	1.54
4	E	62	MET	SD-CE	-5.60	1.65	1.79
3	C	265	PRO	CA-C	5.59	1.54	1.51
4	E	147	ILE	CA-CB	5.48	1.61	1.54
3	C	236	ILE	CA-CB	5.47	1.61	1.54
7	I	4	VAL	CA-CB	5.44	1.61	1.54
5	D	83	ARG	CA-C	5.43	1.57	1.52
10	H	69	VAL	CA-CB	5.38	1.60	1.54
5	D	52	VAL	CA-CB	5.36	1.61	1.54
3	C	243	VAL	CA-CB	5.32	1.61	1.54
3	C	348	ILE	CA-CB	5.23	1.60	1.54
2	B	186	VAL	CA-CB	5.23	1.60	1.54
4	E	194	ILE	CA-CB	5.22	1.60	1.54
4	E	182	VAL	CA-CB	5.21	1.60	1.54
2	B	18	PRO	CA-C	5.21	1.57	1.52
3	C	356	VAL	CA-CB	5.17	1.60	1.54
8	F	16	ILE	CA-CB	5.15	1.60	1.54
3	C	118	ILE	CA-CB	5.13	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	397	THR	CA-CB	5.12	1.62	1.53
1	A	297	ILE	CA-CB	5.10	1.60	1.54
3	C	13	ILE	CA-CB	5.09	1.60	1.54
3	C	190	MET	SD-CE	5.08	1.92	1.79
3	C	138	MET	SD-CE	-5.06	1.67	1.79
2	B	108	THR	CA-CB	5.03	1.61	1.53
1	A	335	MET	SD-CE	-5.02	1.67	1.79
1	A	149	VAL	CA-CB	5.00	1.61	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	VAL	N-CA-C	7.86	115.33	107.55
6	G	50	PRO	N-CA-C	6.79	118.98	110.70
1	A	328	HIS	N-CA-C	6.35	119.02	111.33
3	C	226	ILE	N-CA-C	6.12	116.91	110.72
3	C	265	PRO	O-C-N	5.56	123.87	121.31
2	B	108	THR	N-CA-C	5.54	118.73	110.14
7	I	26	LEU	N-CA-C	5.53	119.20	111.30
3	C	78	ILE	N-CA-CB	5.50	116.99	110.55
4	E	53	ASN	N-CA-C	5.38	116.95	111.14
1	A	281	ASP	N-CA-C	5.28	116.31	108.86
2	B	197	ASN	N-CA-C	5.22	119.74	113.17
5	D	116	ILE	N-CA-C	5.05	117.36	111.05

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	PHE	Peptide
1	A	228	VAL	Peptide
1	A	280	TYR	Peptide
1	A	388	ARG	Peptide
2	B	169	ARG	Peptide
2	B	226	ILE	Peptide
2	B	233	SER	Peptide
2	B	234	GLY	Peptide
2	B	248	ASN	Peptide
2	B	39	GLU	Peptide
2	B	79	GLY	Peptide
3	C	25	SER	Peptide
3	C	270	PRO	Peptide

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Mol	Chain	Res	Type	Group
5	D	115	TYR	Peptide
5	D	144	ARG	Peptide
5	D	145	GLU	Peptide
5	D	53	GLY	Peptide
5	D	73	GLY	Peptide
4	E	188	THR	Peptide
7	I	23	ALA	Peptide
7	I	26	LEU	Peptide
7	I	34	VAL	Peptide
7	I	35	PRO	Peptide
7	I	37	THR	Peptide
7	I	42	VAL	Mainchain,Peptide
7	I	52	ARG	Peptide
11	J	59	TYR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3458	0	3356	26	0
2	B	3172	0	3152	27	0
3	C	3003	0	3065	39	0
4	E	1519	0	1503	4	0
5	D	1919	0	1870	17	0
6	G	628	0	636	3	0
7	I	406	0	437	11	0
8	F	911	0	904	4	0
9	K	438	0	447	6	0
10	H	548	0	530	2	0
11	J	495	0	493	3	0
12	C	23	0	26	4	0
13	C	86	0	64	10	0
13	D	43	0	32	4	0
14	C	37	0	41	5	0
15	E	4	0	0	0	0
16	A	65	0	0	0	0
16	B	99	0	0	2	0
16	C	36	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	D	19	0	0	1	0
16	E	8	0	0	0	0
16	F	32	0	0	0	0
16	G	19	0	0	0	0
16	H	6	0	0	0	0
16	I	2	0	0	0	0
16	K	2	0	0	0	0
All	All	16978	0	16556	132	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 4.

All (132) 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)
2:B:385:GLN:HE22	2:B:393:THR:H	1.11	0.93
5:D:37:CYS:SG	13:D:242:HEC:HAB	2.19	0.82
12:C:380:UQ2:H2M3	13:C:381:HEC:HBA2	1.64	0.78
9:K:38:TRP:CE3	9:K:41:ILE:HD13	2.22	0.74
3:C:94:LEU:HD21	3:C:123:VAL:HG11	1.72	0.72
2:B:100:SER:O	7:I:13:PRO:HD2	1.90	0.72
3:C:21:LEU:HD21	12:C:380:UQ2:H3M3	1.71	0.71
2:B:385:GLN:NE2	2:B:393:THR:H	1.86	0.70
2:B:99:THR:HB	7:I:14:VAL:HG22	1.77	0.66
9:K:38:TRP:CE3	9:K:41:ILE:CD1	2.79	0.66
7:I:43:LEU:HA	7:I:46:LYS:HD3	1.77	0.65
3:C:75:TYR:HB3	3:C:78:ILE:HD11	1.78	0.65
2:B:76:THR:HG22	2:B:82:SER:H	1.62	0.65
8:F:28:LYS:HB3	8:F:74:ILE:HG12	1.81	0.61
13:C:382:HEC:HBC3	13:C:382:HEC:HMC1	1.84	0.58
5:D:47:ALA:H	5:D:50:HIS:CD2	2.21	0.58
3:C:29:SER:HA	3:C:32:ASN:HD22	1.68	0.57
5:D:136:GLU:H	5:D:136:GLU:CD	2.12	0.56
3:C:30:TRP:HZ3	3:C:96:MET:HG3	1.71	0.56
3:C:119:LEU:HD22	13:C:381:HEC:HBB3	1.86	0.56
1:A:341:GLN:HE22	1:A:344:ARG:HE	1.54	0.55
2:B:258:VAL:HG12	2:B:423:SER:HB2	1.89	0.55
2:B:70:ARG:HG3	2:B:98:VAL:HG22	1.88	0.55
3:C:82:MET:HG2	3:C:240:MET:HE1	1.89	0.54
5:D:178:THR:HG23	5:D:181:GLN:HB2	1.89	0.54
4:E:156:TYR:HB2	4:E:165:TYR:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:GLN:HE22	7:I:46:LYS:HG3	1.73	0.54
1:A:75:LEU:HD12	1:A:112:LEU:HD22	1.89	0.53
3:C:197:LEU:HD11	13:C:381:HEC:HMA3	1.91	0.53
5:D:163:PRO:HG2	13:D:242:HEC:HBB2	1.91	0.53
7:I:29:LEU:HA	7:I:32:ALA:HB3	1.91	0.52
1:A:255:ILE:HD13	1:A:335:MET:HE1	1.92	0.52
3:C:206:ASN:HD21	3:C:210:GLY:HA2	1.75	0.52
3:C:94:LEU:HD21	3:C:123:VAL:CG1	2.39	0.52
3:C:45:ILE:HA	13:C:382:HEC:HMC2	1.93	0.51
3:C:186:PRO:HG2	13:C:382:HEC:HMC3	1.93	0.51
5:D:21:LEU:HB3	5:D:26:ILE:HD11	1.93	0.50
2:B:111:CYS:HB3	2:B:119:LEU:HD13	1.94	0.50
1:A:375:VAL:HG13	1:A:389:ARG:HH22	1.76	0.50
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.47	0.50
1:A:25:VAL:HG12	1:A:197:LEU:HB3	1.93	0.50
6:G:73:ASN:HB3	6:G:74:PRO:HD3	1.93	0.49
1:A:430:GLN:O	1:A:430:GLN:HG3	2.12	0.49
3:C:129:MET:HE1	14:C:383:SMA:H41	1.95	0.49
3:C:301:LEU:HA	3:C:304:ILE:HD12	1.93	0.49
9:K:19:PRO:O	9:K:22:SER:OG	2.29	0.49
9:K:48:ILE:HA	11:J:33:ARG:HD3	1.95	0.48
11:J:10:TYR:HA	11:J:14:PHE:HB2	1.95	0.48
3:C:147:THR:HG22	3:C:161:VAL:HG13	1.94	0.48
1:A:131:ARG:NH2	1:A:177:LEU:O	2.47	0.47
4:E:17:GLU:HG3	4:E:28:SER:HB2	1.94	0.47
7:I:40:SER:HA	7:I:41:PRO:HD3	1.86	0.47
1:A:85:HIS:CD2	2:B:370:MET:HE1	2.50	0.47
1:A:145:MET:O	1:A:149:VAL:HG22	2.14	0.47
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.97	0.47
3:C:124:MET:HE3	14:C:383:SMA:H16	1.95	0.47
4:E:158:CYS:HB3	4:E:163:SER:HB2	1.96	0.47
3:C:206:ASN:ND2	3:C:207:ASN:H	2.13	0.46
3:C:276:PHE:HB3	3:C:336:THR:HG22	1.97	0.46
1:A:240:GLN:HG3	1:A:422:VAL:HB	1.98	0.46
2:B:37:SER:HB3	2:B:216:LEU:HD12	1.97	0.46
1:A:85:HIS:HB2	1:A:100:LYS:HB2	1.97	0.46
3:C:277:ALA:HB1	3:C:294:LEU:HD12	1.98	0.46
1:A:252:HIS:CD2	1:A:323:HIS:HE1	2.33	0.46
3:C:133:LEU:HA	3:C:175:LEU:HD21	1.98	0.46
3:C:230:LEU:HD22	5:D:223:LYS:HG2	1.98	0.46
3:C:270:PRO:HA	14:C:383:SMA:H10	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:152:ALA:CB	3:C:291:VAL:HG11	2.45	0.46
3:C:197:LEU:HG	12:C:380:UQ2:H5M3	1.97	0.46
3:C:300:ILE:HD11	3:C:363:LEU:HD13	1.97	0.45
4:E:15:ARG:HD2	4:E:32:ARG:HG2	1.98	0.45
1:A:117:VAL:HG11	1:A:195:MET:HE1	1.98	0.45
2:B:124:LEU:HD11	2:B:219:VAL:HG13	1.99	0.45
3:C:135:TRP:CE3	3:C:175:LEU:HG	2.51	0.45
9:K:33:VAL:HG22	9:K:38:TRP:HE3	1.81	0.45
1:A:308:GLN:HE21	1:A:323:HIS:CD2	2.34	0.45
3:C:77:TRP:CZ3	5:D:201:ARG:HB3	2.52	0.45
9:K:38:TRP:CD2	9:K:41:ILE:CD1	3.00	0.45
2:B:40:ASN:HD22	2:B:40:ASN:C	2.23	0.45
1:A:255:ILE:HG21	1:A:335:MET:HE1	1.99	0.44
5:D:131:LEU:HD11	13:D:242:HEC:HMB3	2.00	0.44
1:A:62:LEU:HD13	1:A:122:LEU:HD23	2.00	0.44
2:B:276:GLN:HE21	2:B:276:GLN:HB3	1.67	0.44
1:A:252:HIS:HE1	7:I:43:LEU:HB3	1.82	0.44
3:C:359:PHE:O	3:C:363:LEU:HB2	2.16	0.44
2:B:309:VAL:HG13	2:B:326:THR:HG22	2.00	0.44
2:B:170:ASN:HD22	2:B:237:ALA:HA	1.83	0.43
2:B:343:GLN:O	2:B:346:THR:HG22	2.18	0.43
1:A:108:LYS:HD3	1:A:108:LYS:HA	1.84	0.43
2:B:78:LYS:HD3	2:B:129:ALA:HB1	2.01	0.43
8:F:53:ASN:HD22	8:F:53:ASN:H	1.65	0.43
13:C:381:HEC:HBC2	13:C:381:HEC:HMC1	2.00	0.43
5:D:37:CYS:SG	13:D:242:HEC:CAB	3.01	0.43
6:G:26:PHE:HB3	6:G:29:TYR:HB2	2.00	0.42
2:B:108:THR:HG23	16:B:593:HOH:O	2.18	0.42
2:B:76:THR:HG21	16:B:589:HOH:O	2.18	0.42
8:F:50:LEU:HD21	8:F:90:LEU:HD23	2.02	0.42
1:A:60:GLU:OE1	2:B:287:ARG:NH2	2.52	0.42
3:C:126:THR:HG21	13:C:382:HEC:HBB3	2.01	0.42
3:C:129:MET:HB3	3:C:182:HIS:HB2	2.01	0.42
16:D:720:HOH:O	11:J:51:LEU:HB3	2.18	0.42
3:C:26:ASN:HD21	8:F:69:SER:CB	2.33	0.42
3:C:332:LEU:O	3:C:336:THR:HG23	2.19	0.42
2:B:209:LEU:HD11	2:B:378:PHE:CD2	2.54	0.42
3:C:186:PRO:HG3	13:C:382:HEC:HBB3	2.02	0.42
3:C:223:TYR:HB3	5:D:227:TRP:CZ2	2.55	0.42
7:I:15:LEU:HD22	7:I:15:LEU:HA	1.86	0.42
1:A:92:ARG:HD3	1:A:163:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:SER:HA	1:A:223:TYR:HB2	2.01	0.42
2:B:313:ASN:HD22	2:B:322:PHE:HD1	1.67	0.42
12:C:380:UQ2:C8	12:C:380:UQ2:H5M1	2.50	0.42
1:A:61:HIS:HB3	1:A:130:GLU:HG3	2.02	0.42
3:C:214:ASP:CG	6:G:2:ARG:HH22	2.28	0.42
5:D:47:ALA:H	5:D:50:HIS:HD2	1.66	0.42
2:B:384:SER:HB2	7:I:2:LEU:O	2.20	0.41
5:D:181:GLN:HG2	10:H:77:LEU:HB3	2.01	0.41
1:A:25:VAL:HG11	1:A:212:ALA:CB	2.51	0.41
5:D:117:VAL:HG11	5:D:191:ARG:HD2	2.01	0.41
1:A:255:ILE:HD13	1:A:335:MET:CE	2.49	0.41
2:B:157:ALA:O	2:B:161:GLU:HG2	2.21	0.41
5:D:163:PRO:HD2	5:D:164:ILE:HG13	2.02	0.41
5:D:118:ARG:HG3	5:D:194:ALA:HB1	2.03	0.41
3:C:270:PRO:HG3	14:C:383:SMA:C8A	2.52	0.40
3:C:270:PRO:HB3	3:C:274:PHE:HB2	2.03	0.40
7:I:43:LEU:HD22	7:I:46:LYS:HE2	2.02	0.40
3:C:8:HIS:HD2	3:C:11:MET:H	1.70	0.40
14:C:383:SMA:H36	14:C:383:SMA:H15	1.94	0.40
2:B:100:SER:O	7:I:13:PRO:CD	2.66	0.40
3:C:25:SER:HA	3:C:218:ILE:HG12	2.03	0.40
13:C:382:HEC:CGD	13:C:382:HEC:HHA	2.51	0.40
1:A:27:SER:HB3	1:A:208:LEU:HD12	2.03	0.40
5:D:132:THR:HG22	10:H:17:LEU:HD22	2.04	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%)	425 (96%)	15 (3%)	4 (1%)	14 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	421/439 (96%)	403 (96%)	16 (4%)	2 (0%)	24	46
3	C	376/379 (99%)	361 (96%)	15 (4%)	0	100	100
4	E	194/196 (99%)	184 (95%)	9 (5%)	1 (0%)	24	46
5	D	239/241 (99%)	223 (93%)	14 (6%)	2 (1%)	16	34
6	G	73/81 (90%)	66 (90%)	5 (7%)	2 (3%)	4	7
7	I	55/78 (70%)	35 (64%)	14 (26%)	6 (11%)	0	0
8	F	103/110 (94%)	102 (99%)	1 (1%)	0	100	100
9	K	51/56 (91%)	47 (92%)	4 (8%)	0	100	100
10	H	65/78 (83%)	63 (97%)	2 (3%)	0	100	100
11	J	58/62 (94%)	53 (91%)	5 (9%)	0	100	100
All	All	2079/2166 (96%)	1962 (94%)	100 (5%)	17 (1%)	16	34

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
1	A	229	PRO
7	I	40	SER
7	I	43	LEU
1	A	286	GLY
2	B	171	ALA
7	I	45	LEU
5	D	95	TYR
6	G	73	ASN
6	G	74	PRO
1	A	232	SER
4	E	70	ALA
5	D	169	LEU
7	I	29	LEU
7	I	51	CYS
7	I	13	PRO
2	B	79	GLY

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%)	321 (87%)	49 (13%)	4	8
2	B	332/343 (97%)	291 (88%)	41 (12%)	4	9
3	C	326/327 (100%)	279 (86%)	47 (14%)	3	6
4	E	168/168 (100%)	140 (83%)	28 (17%)	2	4
5	D	206/206 (100%)	162 (79%)	44 (21%)	1	2
6	G	66/71 (93%)	55 (83%)	11 (17%)	2	4
7	I	44/60 (73%)	26 (59%)	18 (41%)	0	0
8	F	96/98 (98%)	79 (82%)	17 (18%)	2	3
9	K	43/46 (94%)	31 (72%)	12 (28%)	0	1
10	H	64/74 (86%)	44 (69%)	20 (31%)	0	0
11	J	50/52 (96%)	42 (84%)	8 (16%)	2	4
All	All	1765/1815 (97%)	1470 (83%)	295 (17%)	2	4

All (295) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	23	LEU
1	A	32	GLN
1	A	37	VAL
1	A	42	ASP
1	A	50	GLU
1	A	60	GLU
1	A	75	LEU
1	A	77	LYS
1	A	81	SER
1	A	102	LEU
1	A	113	LEU
1	A	121	SER
1	A	122	LEU
1	A	126	GLN
1	A	127	ILE
1	A	146	ARG
1	A	149	VAL
1	A	163	LEU
1	A	176	LYS

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Mol	Chain	Res	Type
1	A	187	SER
1	A	191	LYS
1	A	203	LEU
1	A	208	LEU
1	A	209	LEU
1	A	214	LYS
1	A	219	LEU
1	A	222	THR
1	A	224	ASP
1	A	228	VAL
1	A	230	THR
1	A	245	GLU
1	A	255	ILE
1	A	281	ASP
1	A	300	THR
1	A	302	LYS
1	A	305	GLN
1	A	323	HIS
1	A	350	THR
1	A	351	GLU
1	A	352	SER
1	A	381	ARG
1	A	383	LEU
1	A	388	ARG
1	A	389	ARG
1	A	392	LEU
1	A	409	GLU
1	A	430	GLN
1	A	438	ARG
2	B	17	VAL
2	B	20	HIS
2	B	25	GLU
2	B	38	LEU
2	B	40	ASN
2	B	46	ARG
2	B	69	LEU
2	B	78	LYS
2	B	84	LYS
2	B	95	LYS
2	B	97	SER
2	B	98	VAL
2	B	99	THR

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Mol	Chain	Res	Type
2	B	108	THR
2	B	109	VAL
2	B	118	ILE
2	B	119	LEU
2	B	121	GLU
2	B	123	LEU
2	B	163	LEU
2	B	176	LEU
2	B	186	VAL
2	B	197	ASN
2	B	217	LYS
2	B	222	GLN
2	B	226	ILE
2	B	236	LYS
2	B	257	LEU
2	B	258	VAL
2	B	264	ILE
2	B	273	SER
2	B	305	GLN
2	B	309	VAL
2	B	346	THR
2	B	361	LYS
2	B	371	SER
2	B	379	LEU
2	B	384	SER
2	B	387	LEU
2	B	391	SER
2	B	397	THR
3	C	4	ILE
3	C	12	LYS
3	C	21	LEU
3	C	42	ILE
3	C	46	LEU
3	C	51	LEU
3	C	56	THR
3	C	60	THR
3	C	64	SER
3	C	78	ILE
3	C	94	LEU
3	C	96	MET
3	C	102	LEU
3	C	129	MET

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Mol	Chain	Res	Type
3	C	156	ILE
3	C	160	LEU
3	C	164	ILE
3	C	171	ASP
3	C	175	LEU
3	C	197	LEU
3	C	205	SER
3	C	215	VAL
3	C	241	LEU
3	C	243	VAL
3	C	249	LEU
3	C	254	ASP
3	C	257	THR
3	C	267	HIS
3	C	268	ILE
3	C	269	LYS
3	C	284	ILE
3	C	292	LEU
3	C	306	LEU
3	C	309	THR
3	C	320	LEU
3	C	328	LEU
3	C	336	THR
3	C	343	VAL
3	C	344	GLU
3	C	345	HIS
3	C	350	ILE
3	C	360	LEU
3	C	361	LEU
3	C	363	LEU
3	C	365	LEU
3	C	378	LYS
3	C	379	TRP
4	E	5	ILE
4	E	6	LYS
4	E	12	ASP
4	E	17	GLU
4	E	18	VAL
4	E	22	THR
4	E	23	LYS
4	E	54	VAL
4	E	60	SER

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Mol	Chain	Res	Type
4	E	69	LEU
4	E	71	MET
4	E	75	GLU
4	E	77	LYS
4	E	80	ASP
4	E	85	LYS
4	E	87	MET
4	E	103	LYS
4	E	104	LYS
4	E	106	ILE
4	E	107	ASP
4	E	108	GLN
4	E	112	VAL
4	E	115	SER
4	E	118	ARG
4	E	124	LEU
4	E	129	LYS
4	E	181	GLU
4	E	188	THR
5	D	3	LEU
5	D	13	SER
5	D	15	ARG
5	D	17	LEU
5	D	24	THR
5	D	37	CYS
5	D	42	SER
5	D	43	MET
5	D	55	CYS
5	D	60	GLU
5	D	62	LYS
5	D	66	GLU
5	D	68	VAL
5	D	76	GLU
5	D	82	MET
5	D	106	ASN
5	D	109	LEU
5	D	112	ASP
5	D	113	LEU
5	D	114	SER
5	D	116	ILE
5	D	118	ARG
5	D	124	GLU

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Mol	Chain	Res	Type
5	D	132	THR
5	D	135	CYS
5	D	136	GLU
5	D	143	LEU
5	D	144	ARG
5	D	145	GLU
5	D	147	LEU
5	D	164	ILE
5	D	168	VAL
5	D	169	LEU
5	D	178	THR
5	D	180	SER
5	D	181	GLN
5	D	201	ARG
5	D	203	ARG
5	D	214	LEU
5	D	223	LYS
5	D	226	LYS
5	D	228	SER
5	D	234	LYS
5	D	241	LYS
6	G	2	ARG
6	G	3	GLN
6	G	18	LEU
6	G	24	ARG
6	G	31	SER
6	G	37	VAL
6	G	45	ILE
6	G	53	VAL
6	G	69	SER
6	G	70	LYS
6	G	72	LYS
7	I	7	ARG
7	I	8	SER
7	I	11	PHE
7	I	15	LEU
7	I	16	SER
7	I	20	ARG
7	I	22	VAL
7	I	26	LEU
7	I	27	ARG
7	I	29	LEU

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Mol	Chain	Res	Type
7	I	31	GLN
7	I	37	THR
7	I	39	GLU
7	I	43	LEU
7	I	44	ASP
7	I	45	LEU
7	I	50	LEU
7	I	52	ARG
8	F	6	VAL
8	F	9	SER
8	F	44	LYS
8	F	53	ASN
8	F	59	VAL
8	F	72	GLN
8	F	73	GLN
8	F	74	ILE
8	F	77	LYS
8	F	81	THR
8	F	85	GLU
8	F	90	LEU
8	F	94	LEU
8	F	95	LYS
8	F	99	ARG
8	F	106	GLU
8	F	110	LYS
9	K	1	MET
9	K	2	LEU
9	K	4	ARG
9	K	6	LEU
9	K	9	ARG
9	K	13	LEU
9	K	18	VAL
9	K	32	LEU
9	K	39	ARG
9	K	40	LEU
9	K	51	LYS
9	K	53	LYS
10	H	13	LEU
10	H	18	THR
10	H	23	GLN
10	H	26	GLN
10	H	27	LEU

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Mol	Chain	Res	Type
10	H	28	GLU
10	H	32	LYS
10	H	35	GLU
10	H	36	ARG
10	H	37	LEU
10	H	38	GLU
10	H	39	LEU
10	H	47	ARG
10	H	49	GLN
10	H	51	GLU
10	H	56	GLU
10	H	60	ASP
10	H	65	ARG
10	H	72	LYS
10	H	78	LYS
11	J	5	LEU
11	J	9	LEU
11	J	46	ILE
11	J	51	LEU
11	J	53	LYS
11	J	55	ILE
11	J	58	LYS
11	J	60	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	18	GLN
1	A	94	HIS
1	A	136	GLN
1	A	207	GLN
1	A	215	HIS
1	A	252	HIS
1	A	274	ASN
1	A	308	GLN
1	A	311	ASN
1	A	323	HIS
1	A	341	GLN
1	A	359	ASN
1	A	418	GLN
2	B	143	GLN

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Mol	Chain	Res	Type
2	B	153	GLN
2	B	162	ASN
2	B	170	ASN
2	B	174	ASN
2	B	197	ASN
2	B	218	GLN
2	B	248	ASN
2	B	270	ASN
2	B	276	GLN
2	B	277	HIS
2	B	284	HIS
2	B	313	ASN
2	B	342	ASN
2	B	351	ASN
2	B	362	ASN
2	B	385	GLN
2	B	429	ASN
3	C	8	HIS
3	C	32	ASN
3	C	54	HIS
3	C	74	ASN
3	C	114	ASN
3	C	137	GLN
3	C	206	ASN
3	C	312	GLN
3	C	322	GLN
5	D	50	HIS
5	D	71	GLN
5	D	121	HIS
5	D	166	ASN
6	G	36	ASN
6	G	73	ASN
7	I	31	GLN
8	F	22	ASN
8	F	53	ASN
9	K	12	GLN
9	K	16	ASN
9	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 [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
15	FES	E	200	4	0,4,4	-	-	-		
13	HEC	C	381	3	50,50,50	1.39	8 (16%)	68,82,82	1.95	18 (26%)
13	HEC	D	242	5	50,50,50	1.34	6 (12%)	68,82,82	1.87	16 (23%)
13	HEC	C	382	3	50,50,50	1.35	7 (14%)	68,82,82	1.87	14 (20%)
12	UQ2	C	380	-	23,23,23	2.72	6 (26%)	30,31,31	1.24	3 (10%)
14	SMA	C	383	-	38,38,38	1.29	3 (7%)	47,52,52	2.07	13 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	FES	E	200	4	-	-	0/1/1/1
13	HEC	C	381	3	-	9/14/54/54	-
13	HEC	D	242	5	1/1/3/7	4/14/54/54	-
13	HEC	C	382	3	1/1/3/7	9/14/54/54	-
12	UQ2	C	380	-	-	3/15/39/39	0/1/1/1
14	SMA	C	383	-	-	14/34/34/34	0/2/2/2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	380	UQ2	C6-C5	9.61	1.52	1.35
14	C	383	SMA	C3-C2	4.57	1.43	1.34
12	C	380	UQ2	C3-C2	4.11	1.51	1.36
13	C	381	HEC	CBA-CGA	-4.07	1.41	1.50
13	C	382	HEC	CBA-CGA	-4.03	1.41	1.50
12	C	380	UQ2	C8-C9	3.87	1.42	1.33
13	D	242	HEC	CBA-CGA	-3.66	1.42	1.50
13	D	242	HEC	CBD-CGD	-3.65	1.42	1.50
13	C	381	HEC	CBD-CGD	-3.64	1.42	1.50
12	C	380	UQ2	C13-C14	3.15	1.41	1.32
12	C	380	UQ2	C7-C8	3.12	1.55	1.50
13	C	382	HEC	CBD-CGD	-3.03	1.43	1.50
13	D	242	HEC	FE-NA	2.97	2.05	1.95
13	C	381	HEC	CHD-C4C	2.89	1.45	1.39
13	C	382	HEC	CHD-C4C	2.66	1.45	1.39
13	C	382	HEC	FE-NB	2.62	2.03	1.94
13	C	382	HEC	FE-NA	2.58	2.03	1.95
13	C	381	HEC	FE-NB	2.56	2.02	1.94
12	C	380	UQ2	C7-C6	2.52	1.56	1.51
13	D	242	HEC	FE-NB	2.52	2.02	1.94
13	C	381	HEC	FE-NA	2.46	2.03	1.95
13	D	242	HEC	CHD-C4C	2.40	1.44	1.39
13	C	382	HEC	FE-ND	2.28	2.01	1.94
14	C	383	SMA	C4A-C5	2.26	1.44	1.40
13	C	381	HEC	FE-ND	2.24	2.01	1.94
14	C	383	SMA	C6-C5	2.18	1.42	1.38
13	D	242	HEC	FE-ND	2.15	2.01	1.94
13	C	381	HEC	O2A-CGA	-2.09	1.23	1.30
13	C	382	HEC	FE-NC	2.05	2.01	1.95
13	C	381	HEC	FE-NC	2.02	2.01	1.95

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	383	SMA	O7-C7-C8	6.53	121.36	114.53
13	D	242	HEC	CHB-C4A-NA	5.97	130.96	124.45
13	C	381	HEC	C2A-C1A-NA	-5.59	104.93	110.32
13	C	382	HEC	CHB-C4A-NA	5.50	130.45	124.45
13	C	382	HEC	CHA-C1A-NA	5.23	130.15	124.45
13	D	242	HEC	CHA-C1A-NA	4.71	129.58	124.45
13	C	382	HEC	C2A-C1A-NA	-4.31	106.17	110.32
13	C	381	HEC	CHB-C4A-NA	4.30	129.13	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D	242	HEC	C2A-C1A-NA	-4.28	106.20	110.32
13	D	242	HEC	CHB-C1B-NB	4.13	128.87	124.42
13	C	381	HEC	C4A-CHB-C1B	-4.08	117.34	126.02
13	C	381	HEC	CHA-C1A-NA	4.00	128.80	124.45
14	C	383	SMA	C22-C11-C10	3.99	116.52	110.34
13	C	382	HEC	C4A-NA-C1A	3.97	112.30	105.82
13	C	381	HEC	C4A-NA-C1A	3.94	112.24	105.82
14	C	383	SMA	O5-C5-C4A	3.88	121.34	115.84
14	C	383	SMA	O14-C14-C13	3.79	115.80	107.97
14	C	383	SMA	O1-C2-C3	-3.67	118.59	121.81
13	C	381	HEC	C4C-CHD-C1D	-3.66	117.64	126.25
13	D	242	HEC	CHD-C1D-ND	3.51	128.71	124.37
13	D	242	HEC	C4A-NA-C1A	3.47	111.48	105.82
13	C	382	HEC	C4A-CHB-C1B	-3.30	119.01	126.02
13	C	382	HEC	CHD-C1D-ND	3.29	128.44	124.37
13	C	382	HEC	C1C-CHC-C4B	-3.23	118.65	126.25
13	C	382	HEC	CHB-C1B-NB	3.22	127.88	124.42
13	C	381	HEC	CHD-C1D-ND	3.21	128.34	124.37
13	D	242	HEC	C4A-CHB-C1B	-3.21	119.20	126.02
14	C	383	SMA	C17-C18-C19	-3.19	117.61	126.36
13	C	382	HEC	C4C-CHD-C1D	-3.17	118.78	126.25
13	C	381	HEC	CAA-C2A-C3A	-3.17	121.93	127.87
13	D	242	HEC	C4C-CHD-C1D	-3.11	118.93	126.25
14	C	383	SMA	O1-C2-C9	3.10	116.70	110.12
13	D	242	HEC	C1C-CHC-C4B	-3.01	119.17	126.25
14	C	383	SMA	O5-C5-C6	-2.93	119.02	124.08
14	C	383	SMA	C25-O14-C14	2.91	119.66	112.99
14	C	383	SMA	O12-C12-C13	2.79	112.08	107.97
14	C	383	SMA	O7-C7-C6	-2.77	119.31	124.08
13	C	381	HEC	C1C-CHC-C4B	-2.69	119.92	126.25
13	D	242	HEC	C1A-CHA-C4D	-2.66	120.36	126.02
13	D	242	HEC	CHA-C4D-ND	2.66	127.28	124.42
13	C	381	HEC	CAA-C2A-C1A	2.65	130.24	124.85
13	C	381	HEC	O2D-CGD-CBD	2.62	122.29	114.00
13	C	381	HEC	CAC-C3C-C2C	2.61	131.02	126.89
13	C	381	HEC	C3A-C4A-NA	-2.54	104.93	109.64
13	C	382	HEC	C3A-C4A-NA	-2.48	105.05	109.64
13	C	381	HEC	CHB-C1B-NB	2.44	127.05	124.42
13	C	382	HEC	C1A-CHA-C4D	-2.43	120.85	126.02
13	D	242	HEC	CHD-C4C-NC	2.38	128.18	123.86
13	C	382	HEC	O2D-CGD-CBD	2.36	121.45	114.00
12	C	380	UQ2	C5-C6-C1	-2.32	117.36	119.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	381	HEC	CHC-C1C-NC	2.31	128.05	123.86
13	D	242	HEC	CHC-C1C-NC	2.27	127.97	123.86
14	C	383	SMA	C6-C7-C8	-2.26	118.44	120.59
13	C	381	HEC	C1A-CHA-C4D	-2.25	121.25	126.02
12	C	380	UQ2	C6-C5-C4	2.22	120.92	119.17
13	C	381	HEC	CHC-C4B-NB	2.22	127.11	124.37
13	C	382	HEC	CHD-C4C-NC	2.17	127.79	123.86
13	D	242	HEC	CHC-C4B-NB	2.13	127.00	124.37
13	C	381	HEC	CBC-CAC-C3C	2.13	118.19	112.42
12	C	380	UQ2	C10-C9-C11	2.12	118.91	115.23
13	D	242	HEC	CHB-C1B-C2B	-2.10	121.71	125.03
13	C	382	HEC	CHA-C4D-ND	2.06	126.64	124.42
13	D	242	HEC	C3A-C4A-NA	-2.05	105.85	109.64
14	C	383	SMA	C24-C13-C14	2.03	115.06	110.95

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	C	382	HEC	NA
13	D	242	HEC	NA

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	C	381	HEC	C2C-C3C-CAC-CBC
13	C	382	HEC	C4C-C3C-CAC-CBC
13	C	381	HEC	C4C-C3C-CAC-CBC
13	C	381	HEC	C1A-C2A-CAA-CBA
13	C	382	HEC	C2C-C3C-CAC-CBC
14	C	383	SMA	C8-C7-O7-C7M
14	C	383	SMA	C6-C5-O5-C5M
14	C	383	SMA	C6-C7-O7-C7M
13	C	381	HEC	C3A-C2A-CAA-CBA
14	C	383	SMA	C4A-C5-O5-C5M
14	C	383	SMA	C24-C13-C14-C15
14	C	383	SMA	C24-C13-C14-O14
14	C	383	SMA	C12-C13-C14-O14
14	C	383	SMA	C13-C14-O14-C25
14	C	383	SMA	C9-C10-C11-C22
13	C	382	HEC	C3D-CAD-CBD-CGD
12	C	380	UQ2	C5-C6-C7-C8
14	C	383	SMA	O1-C2-C9-C10

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Mol	Chain	Res	Type	Atoms
12	C	380	UQ2	C1-C6-C7-C8
12	C	380	UQ2	C2-C3-O3-CM3
13	C	382	HEC	C4B-C3B-CAB-CBB
13	C	381	HEC	C2A-CAA-CBA-CGA
13	C	382	HEC	CAA-CBA-CGA-O2A
13	D	242	HEC	CAA-CBA-CGA-O1A
14	C	383	SMA	C15-C14-O14-C25
13	C	381	HEC	CAA-CBA-CGA-O2A
13	C	382	HEC	CAD-CBD-CGD-O1D
13	C	382	HEC	CAA-CBA-CGA-O1A
13	C	382	HEC	C2B-C3B-CAB-CBB
13	D	242	HEC	CAA-CBA-CGA-O2A
13	D	242	HEC	CAD-CBD-CGD-O2D
13	D	242	HEC	CAD-CBD-CGD-O1D
13	C	381	HEC	CAA-CBA-CGA-O1A
13	C	382	HEC	CAD-CBD-CGD-O2D
14	C	383	SMA	O14-C14-C15-C16
14	C	383	SMA	C3-C2-C9-C10
14	C	383	SMA	C11-C10-C9-C2
13	C	381	HEC	CAD-CBD-CGD-O2D
13	C	381	HEC	C4B-C3B-CAB-CBB

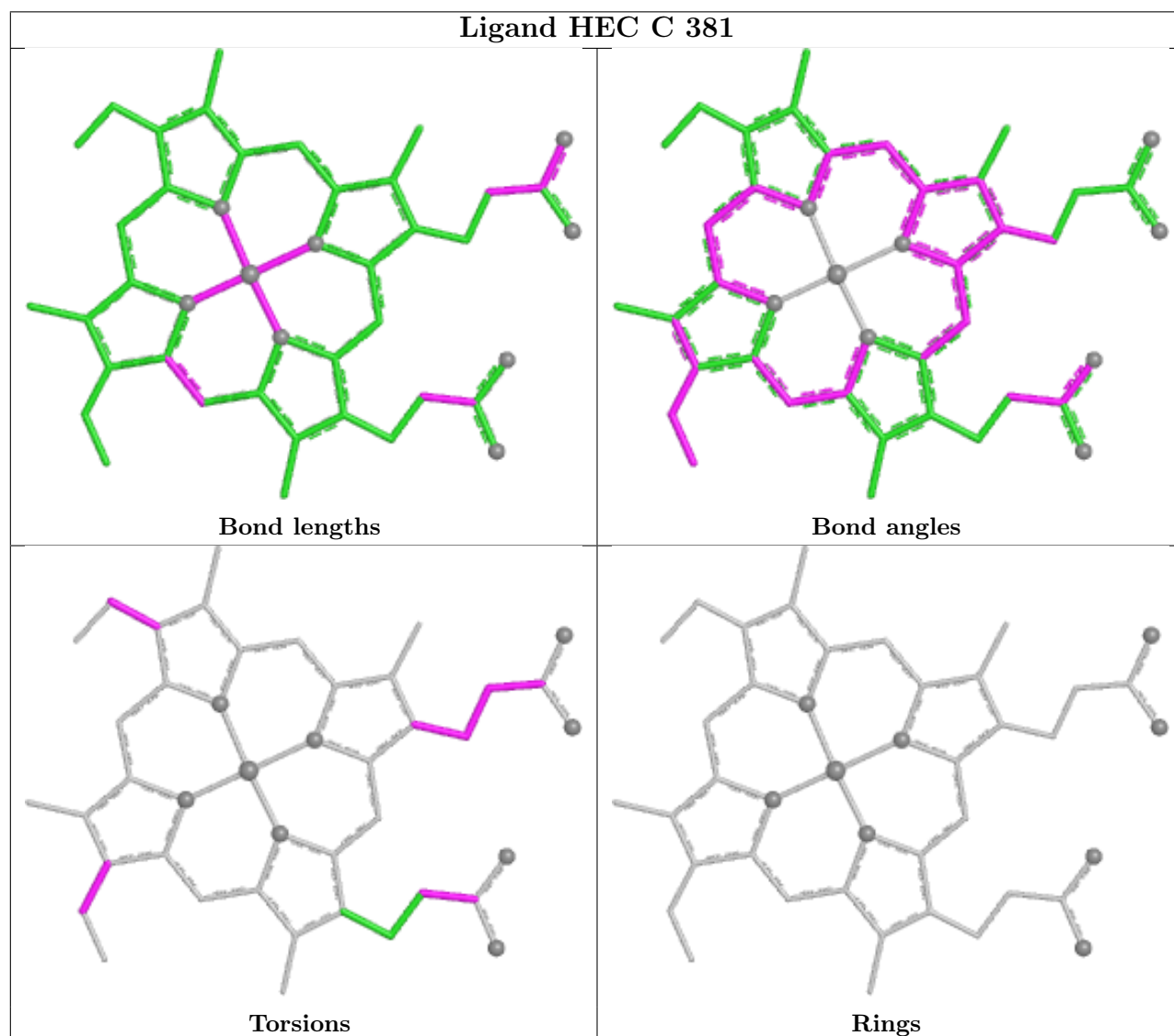
There are no ring outliers.

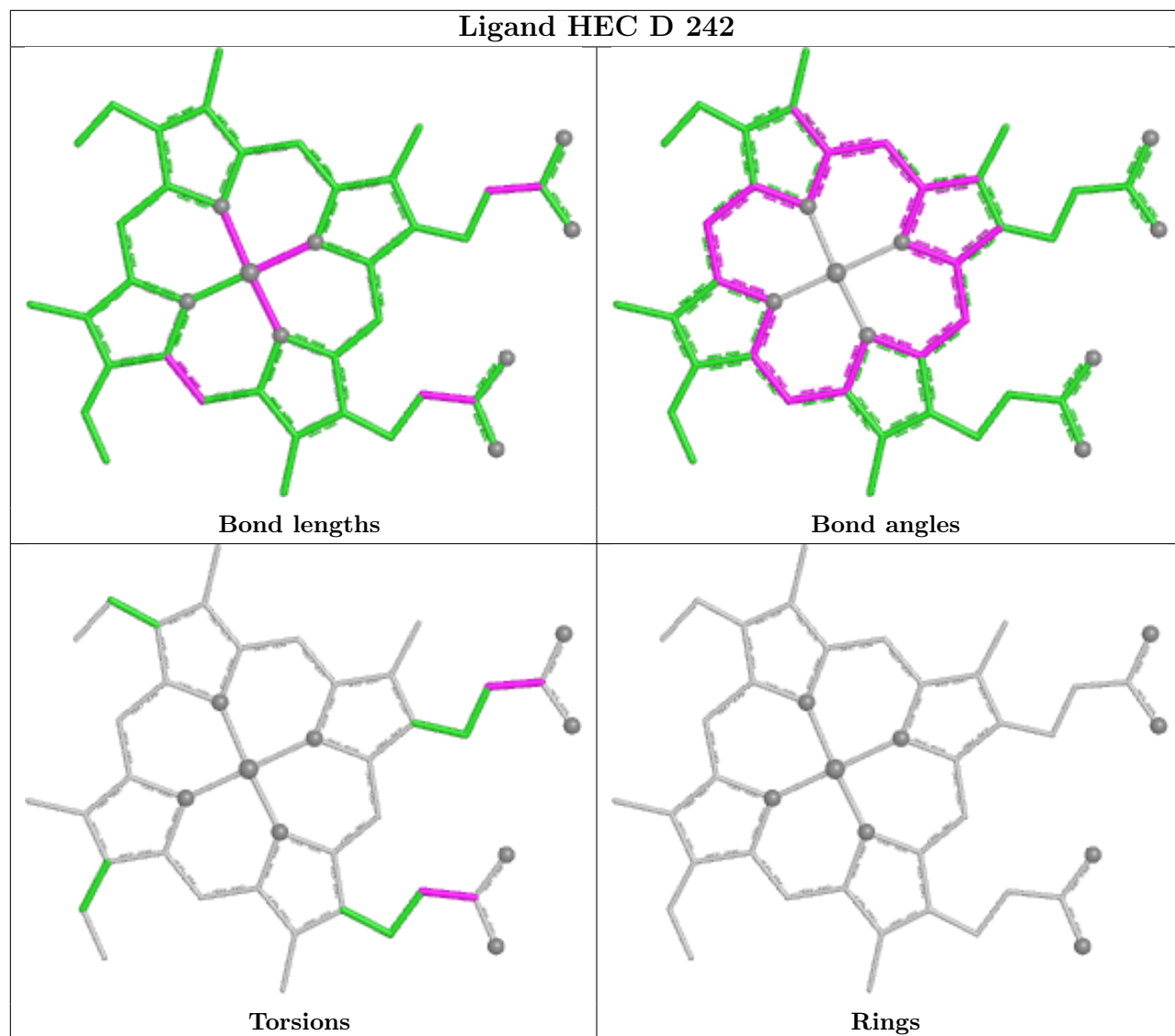
5 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	381	HEC	4	0
13	D	242	HEC	4	0
13	C	382	HEC	6	0
12	C	380	UQ2	4	0
14	C	383	SMA	5	0

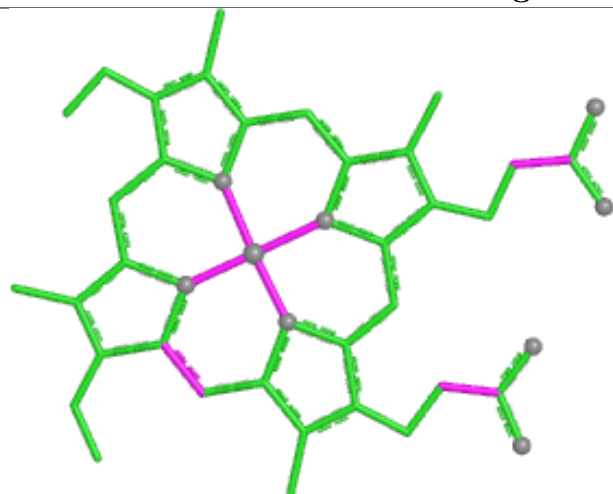
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

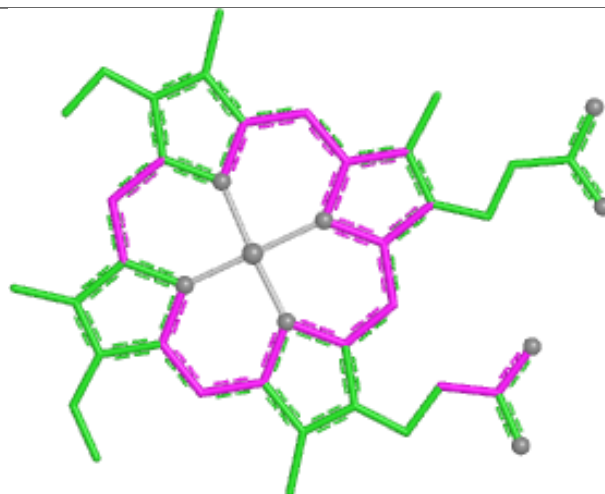




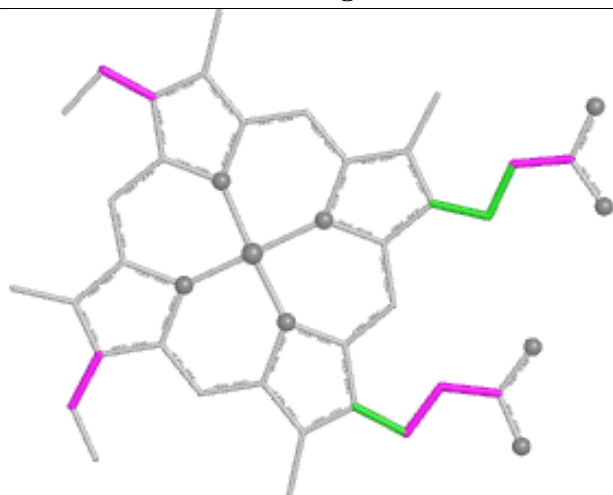
Ligand HEC C 382



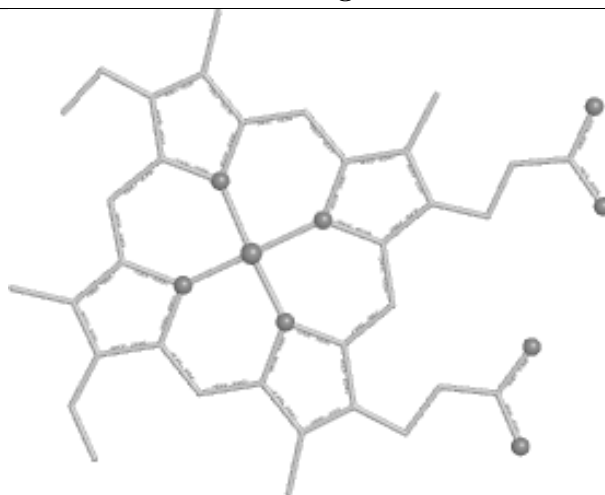
Bond lengths



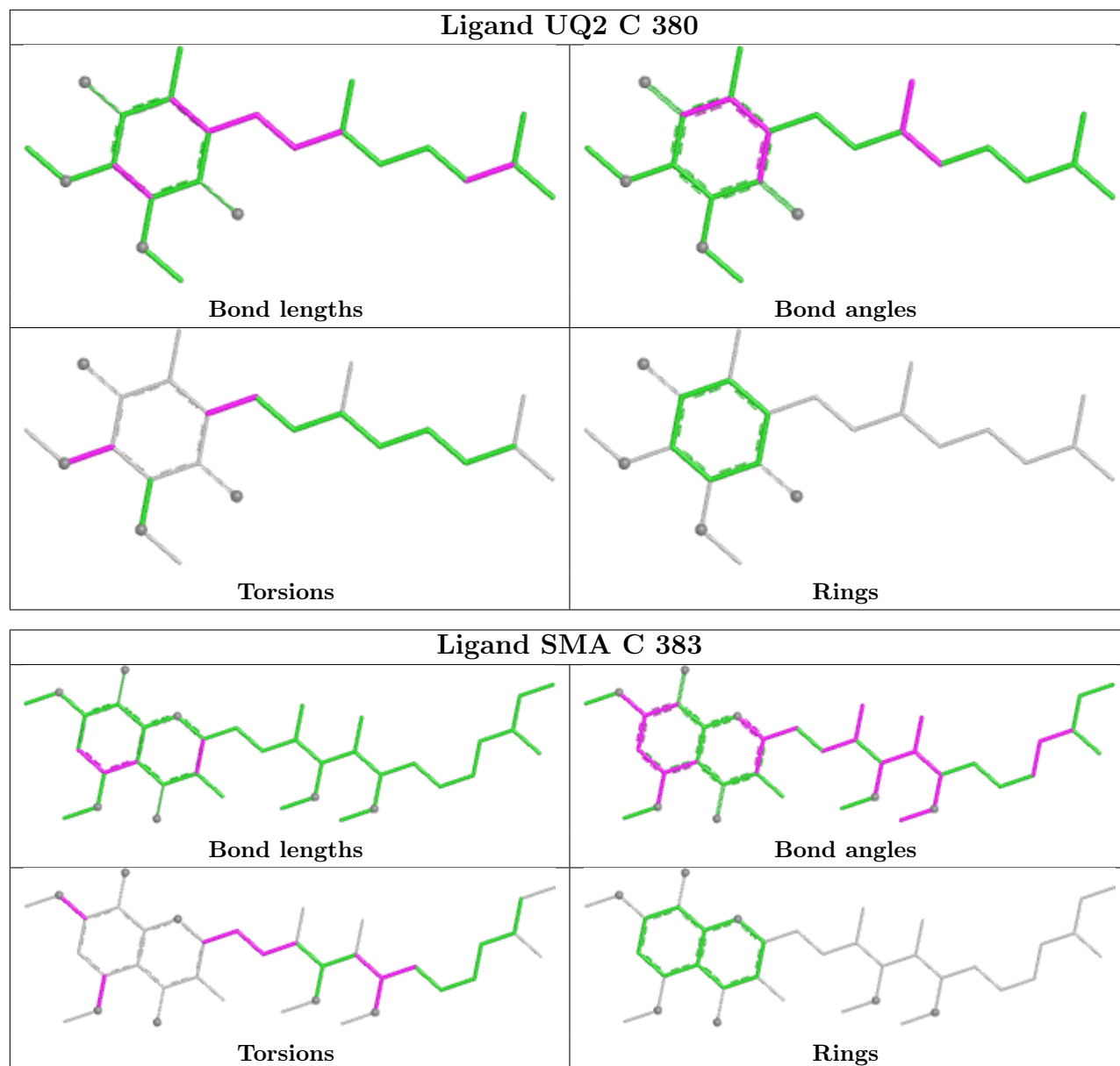
Bond angles



Torsions



Rings



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.