



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 11:37 AM UTC

PDB ID : 1BE3 / pdb\_00001be3  
Title : CYTOCHROME BC1 COMPLEX FROM BOVINE  
Authors : Iwata, S.; Lee, J.W.; Okada, K.; Lee, J.K.; Iwata, M.; Ramaswamy, S.; Jap, B.K.  
Deposited on : 1998-05-19  
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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)  
Xtrriage (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) : 2.49

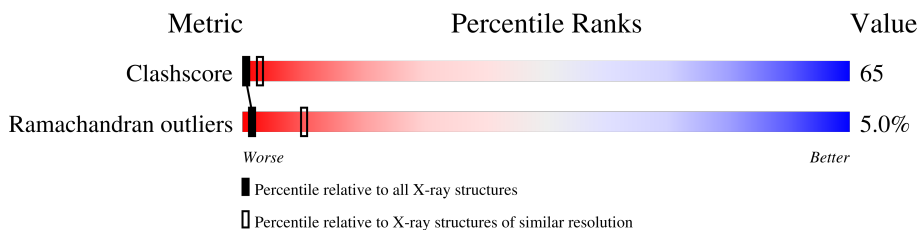
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)

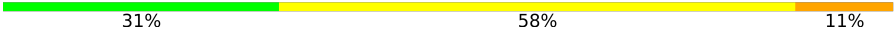

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	446	
2	B	439	
3	C	379	
4	D	241	
5	E	196	
6	F	110	
7	G	81	
8	H	78	
9	I	78	

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Mol	Chain	Length	Quality of chain
10	J	62	 31% 58% 11%
11	K	56	 12% 21% 5% 61%

## 2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 16222 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 CYTOCHROME BC1 COMPLEX.

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

- Molecule 2 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	419	3141	1972	556	606	7	0	0	0

- Molecule 3 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	379	3011	2018	472	502	19	0	0	0

- Molecule 4 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	241	1919	1225	330	349	15	0	0	0

- Molecule 5 is a protein called CYTOCHROME BC1 COMPLEX.

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

- Molecule 6 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	106	916	579	166	169	2	0	0	0

- Molecule 7 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	81	682	441	128	112	1	0	0	0

- Molecule 8 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	64	524	316	96	107	5	0	0	0

- Molecule 9 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	33	248	152	51	44	1	0	0	0

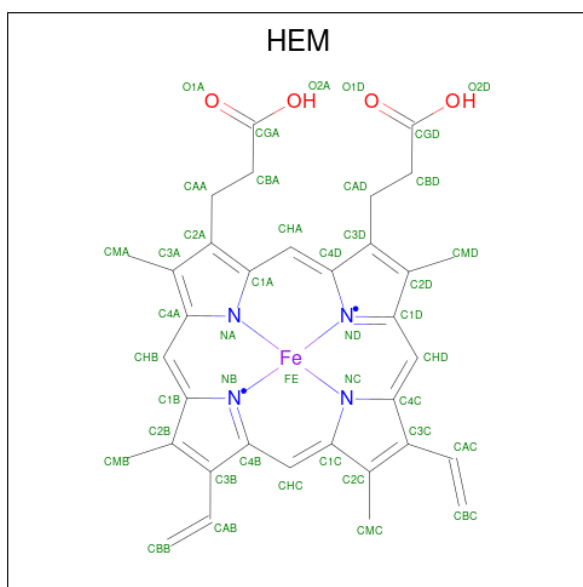
- Molecule 10 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	J	62	512	335	89	88	0	0	0

- Molecule 11 is a protein called CYTOCHROME BC1 COMPLEX.

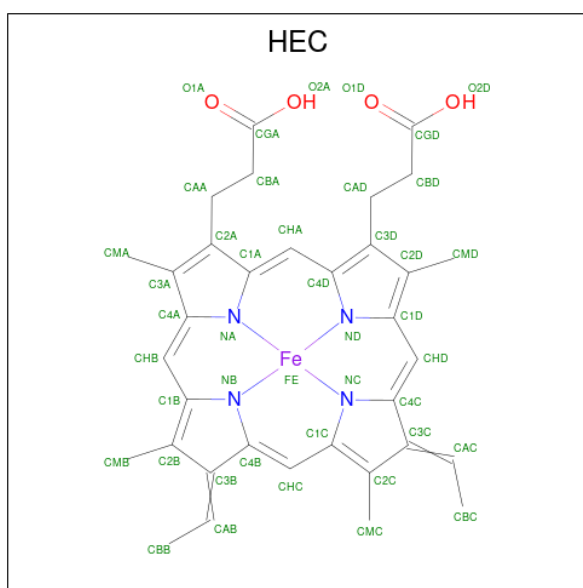
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
11	K	22	159	103	29	27	0	0	0

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



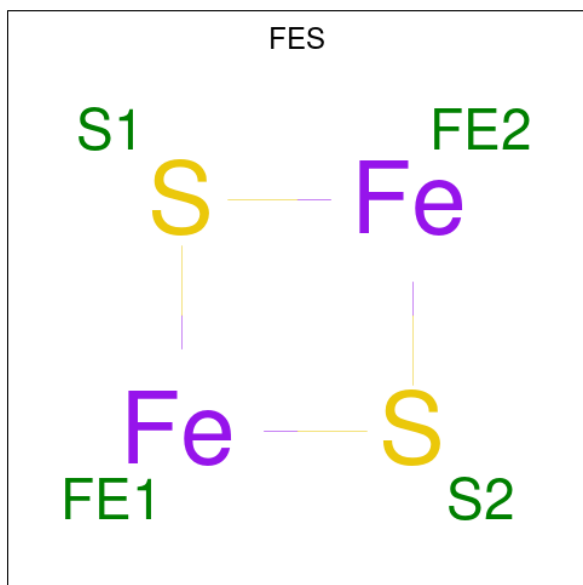
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



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

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $Fe_2S_2$ ).



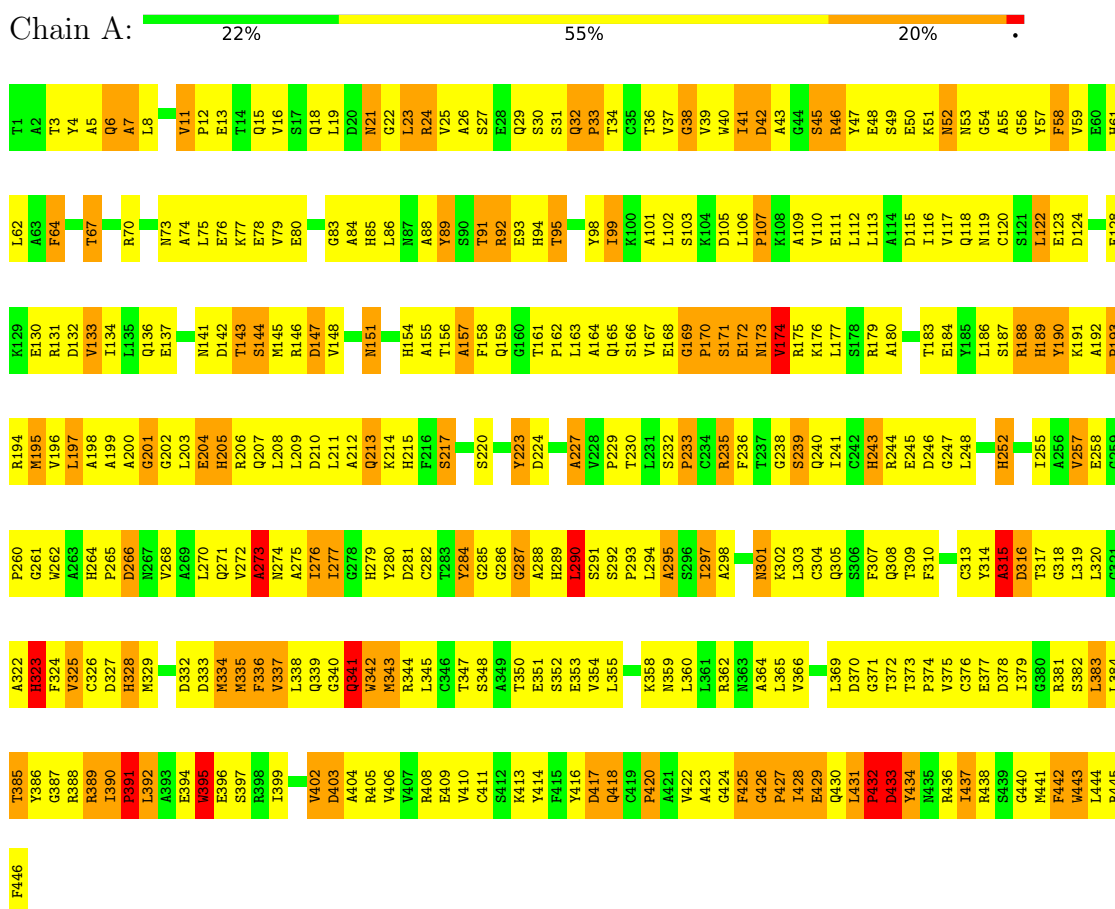
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
14	E	1	4	2	2	0	0

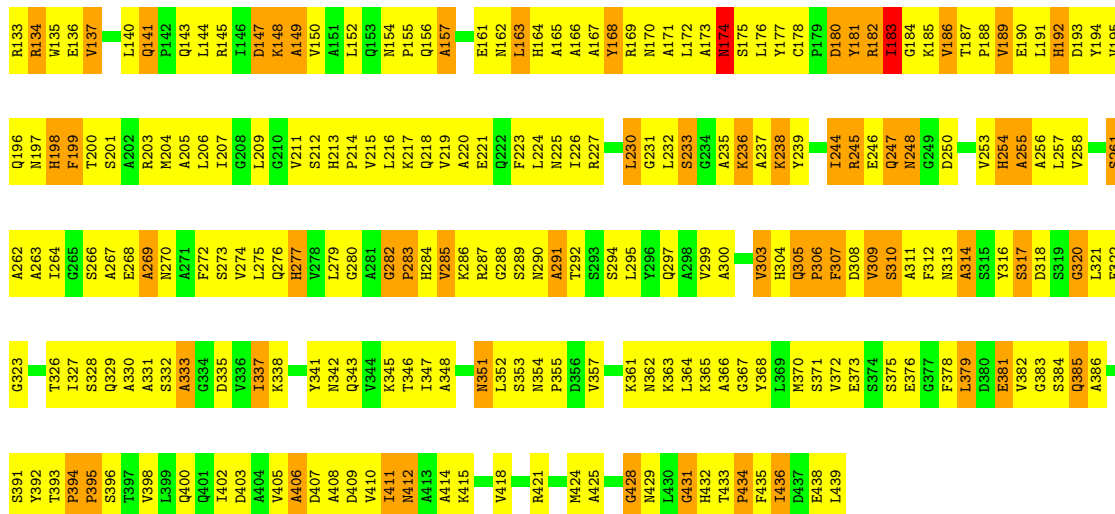
### 3 Residue-property plots [i](#)

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

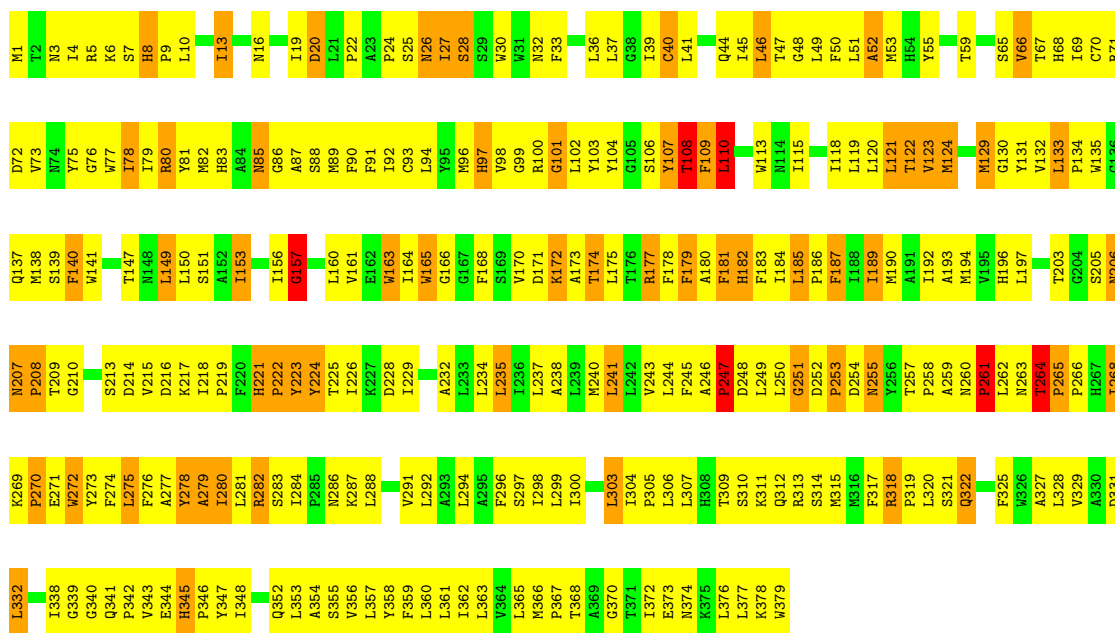
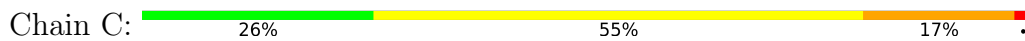
Note EDS was not executed.

- Molecule 1: CYTOCHROME BC1 COMPLEX

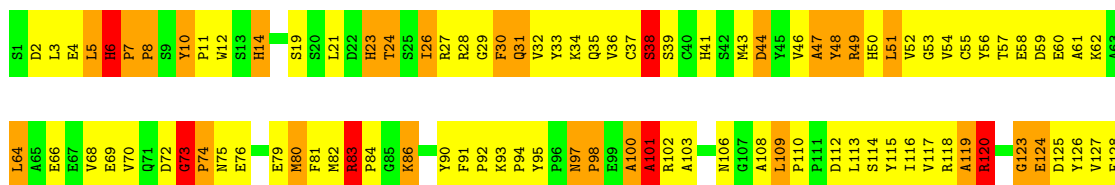


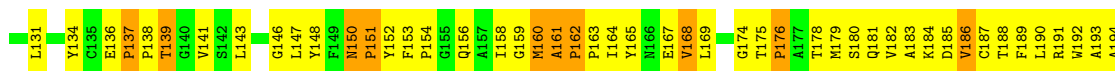


● Molecule 3: CYTOCHROME BC1 COMPLEX



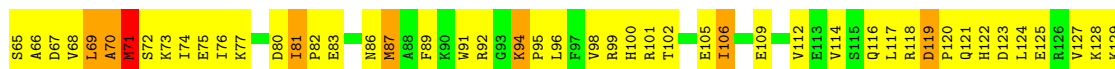
● Molecule 4: CYTOCHROME BC1 COMPLEX





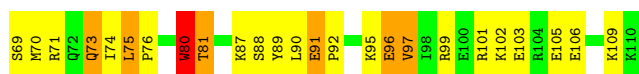
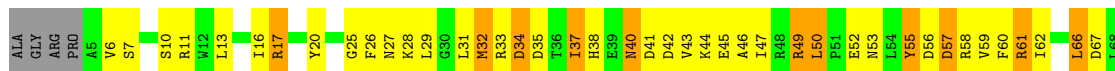
• Molecule 5: CYTOCHROME BC1 COMPLEX

Chain E: 24% 59% 17%



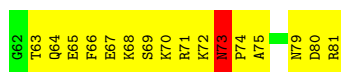
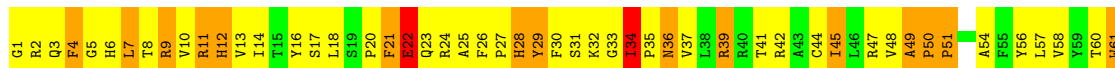
• Molecule 6: CYTOCHROME BC1 COMPLEX

Chain F: 35% 45% 15%



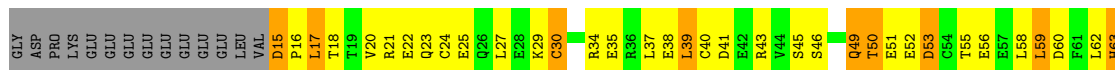
• Molecule 7: CYTOCHROME BC1 COMPLEX

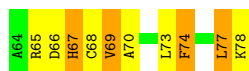
Chain G: 17% 60% 19%



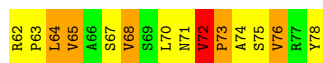
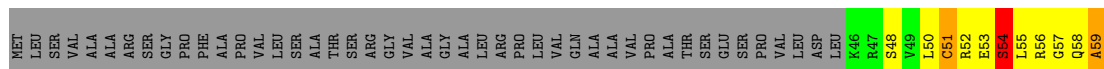
• Molecule 8: CYTOCHROME BC1 COMPLEX

Chain H: 24% 41% 17% 18%

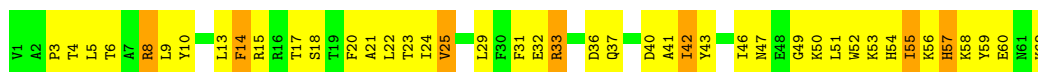




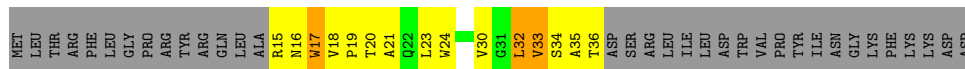
- Molecule 9: CYTOCHROME BC1 COMPLEX



- Molecule 10: CYTOCHROME BC1 COMPLEX



- Molecule 11: CYTOCHROME BC1 COMPLEX



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.20Å 211.20Å 339.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.00	Depositor
% Data completeness (in resolution range)	81.7 (40.00-3.00)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.260 , 0.320	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16222	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: FES, HEC, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.82	6/3531 (0.2%)	2.10	151/4792 (3.2%)
2	B	0.78	4/3198 (0.1%)	2.03	100/4336 (2.3%)
3	C	0.88	8/3108 (0.3%)	2.00	96/4252 (2.3%)
4	D	0.73	4/1978 (0.2%)	1.84	54/2684 (2.0%)
5	E	0.72	2/1553 (0.1%)	1.92	52/2100 (2.5%)
6	F	0.70	0/935	2.00	29/1253 (2.3%)
7	G	0.78	1/704 (0.1%)	1.95	30/951 (3.2%)
8	H	0.74	4/529 (0.8%)	1.58	9/708 (1.3%)
9	I	0.78	0/250	2.07	11/335 (3.3%)
10	J	0.71	1/525 (0.2%)	1.68	12/707 (1.7%)
11	K	0.67	0/163	1.66	1/225 (0.4%)
All	All	0.79	30/16474 (0.2%)	1.98	545/22343 (2.4%)

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	14
2	B	0	17
3	C	0	8
4	D	0	5
5	E	0	5
6	F	0	5
7	G	0	2
8	H	0	1
All	All	0	57

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	LEU	C-O	8.77	1.34	1.23
3	C	174	THR	N-CA	-8.29	1.36	1.46
7	G	79	ASN	C-O	-8.13	1.15	1.23
3	C	280	ILE	CA-CB	-8.01	1.43	1.54
3	C	98	VAL	N-CA	-7.94	1.36	1.46

The worst 5 of 545 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	196	HIS	CA-CB-CG	13.98	127.78	113.80
3	C	265	PRO	CB-CA-C	13.07	126.87	110.92
3	C	206	ASN	OD1-CG-ND2	12.37	134.97	122.60
1	A	268	VAL	N-CA-C	-12.07	100.89	112.96
5	E	182	VAL	N-CA-C	11.03	118.47	107.55

There are no chirality outliers.

5 of 57 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	THR	Mainchain
1	A	190	TYR	Mainchain
1	A	197	LEU	Mainchain
1	A	210	ASP	Mainchain
1	A	47	TYR	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	511	0
2	B	3141	0	3123	421	1
3	C	3011	0	3077	409	2
4	D	1919	0	1868	313	0
5	E	1519	0	1503	193	2
6	F	916	0	909	90	0
7	G	682	0	679	107	0
8	H	524	0	504	60	0
9	I	248	0	265	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	512	0	518	71	0
11	K	159	0	159	23	0
12	C	86	0	60	19	0
13	D	43	0	30	3	0
14	E	4	0	0	1	0
All	All	16222	0	16051	2085	3

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 65.

The worst 5 of 2085 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)
1:A:158:PHE:CE1	1:A:317:THR:HG21	1.71	1.26
1:A:21:ASN:CB	1:A:217:SER:HB2	1.70	1.20
1:A:392:LEU:HA	1:A:395:TRP:CD1	1.79	1.17
2:B:29:LEU:HD12	2:B:33:LEU:HD21	1.19	1.15
1:A:158:PHE:HE1	1:A:317:THR:HG21	0.97	1.12

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:264:THR:OG1	5:E:141:HIS:O[10_665]	1.93	0.27
2:B:169:ARG:NH2	2:B:438:GLU:OE2[10_665]	1.99	0.21
3:C:177:ARG:NH2	5:E:62:MET:O[10_665]	2.12	0.08

## 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%)	359 (81%)	65 (15%)	20 (4%)	2	12
2	B	417/439 (95%)	360 (86%)	43 (10%)	14 (3%)	3	17
3	C	377/379 (100%)	300 (80%)	55 (15%)	22 (6%)	1	8
4	D	239/241 (99%)	188 (79%)	32 (13%)	19 (8%)	1	3
5	E	194/196 (99%)	144 (74%)	40 (21%)	10 (5%)	1	9
6	F	104/110 (94%)	89 (86%)	14 (14%)	1 (1%)	12	45
7	G	79/81 (98%)	57 (72%)	18 (23%)	4 (5%)	1	10
8	H	62/78 (80%)	46 (74%)	11 (18%)	5 (8%)	1	3
9	I	31/78 (40%)	17 (55%)	9 (29%)	5 (16%)	0	0
10	J	60/62 (97%)	47 (78%)	13 (22%)	0	100	100
11	K	20/56 (36%)	15 (75%)	3 (15%)	2 (10%)	0	2
All	All	2027/2166 (94%)	1622 (80%)	303 (15%)	102 (5%)	1	10

5 of 102 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	PRO
1	A	432	PRO
2	B	183	ILE
3	C	8	HIS
3	C	27	ILE

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA [i](#)

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](#)

4 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	HEM	C	380	3	50,50,50	1.27	6 (12%)	67,82,82	1.26	6 (8%)
13	HEC	D	242	4	46,50,50	1.87	7 (15%)	58,82,82	1.44	7 (12%)
12	HEM	C	381	3	50,50,50	1.17	4 (8%)	67,82,82	1.51	14 (20%)
14	FES	E	197	5	0,4,4	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	HEM	C	380	3	-	5/14/54/54	-
13	HEC	D	242	4	-	10/14/54/54	-
12	HEM	C	381	3	-	5/14/54/54	-
14	FES	E	197	5	-	-	0/1/1/1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	242	HEC	CAB-C3B	6.42	1.55	1.35
13	D	242	HEC	CAC-C3C	6.32	1.55	1.35
13	D	242	HEC	CBB-CAB	-4.06	1.34	1.49
13	D	242	HEC	CBC-CAC	-3.70	1.35	1.49
12	C	380	HEM	FE-NB	3.39	2.05	1.94

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D	242	HEC	CBC-CAC-C3C	-6.00	115.44	127.43
13	D	242	HEC	CBB-CAB-C3B	-4.03	119.39	127.43

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	380	HEM	CBD-CAD-C3D	3.97	123.52	112.53
12	C	381	HEM	C4C-C3C-C2C	3.50	109.85	106.81
12	C	381	HEM	C3D-C4D-ND	-3.48	106.35	110.17

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

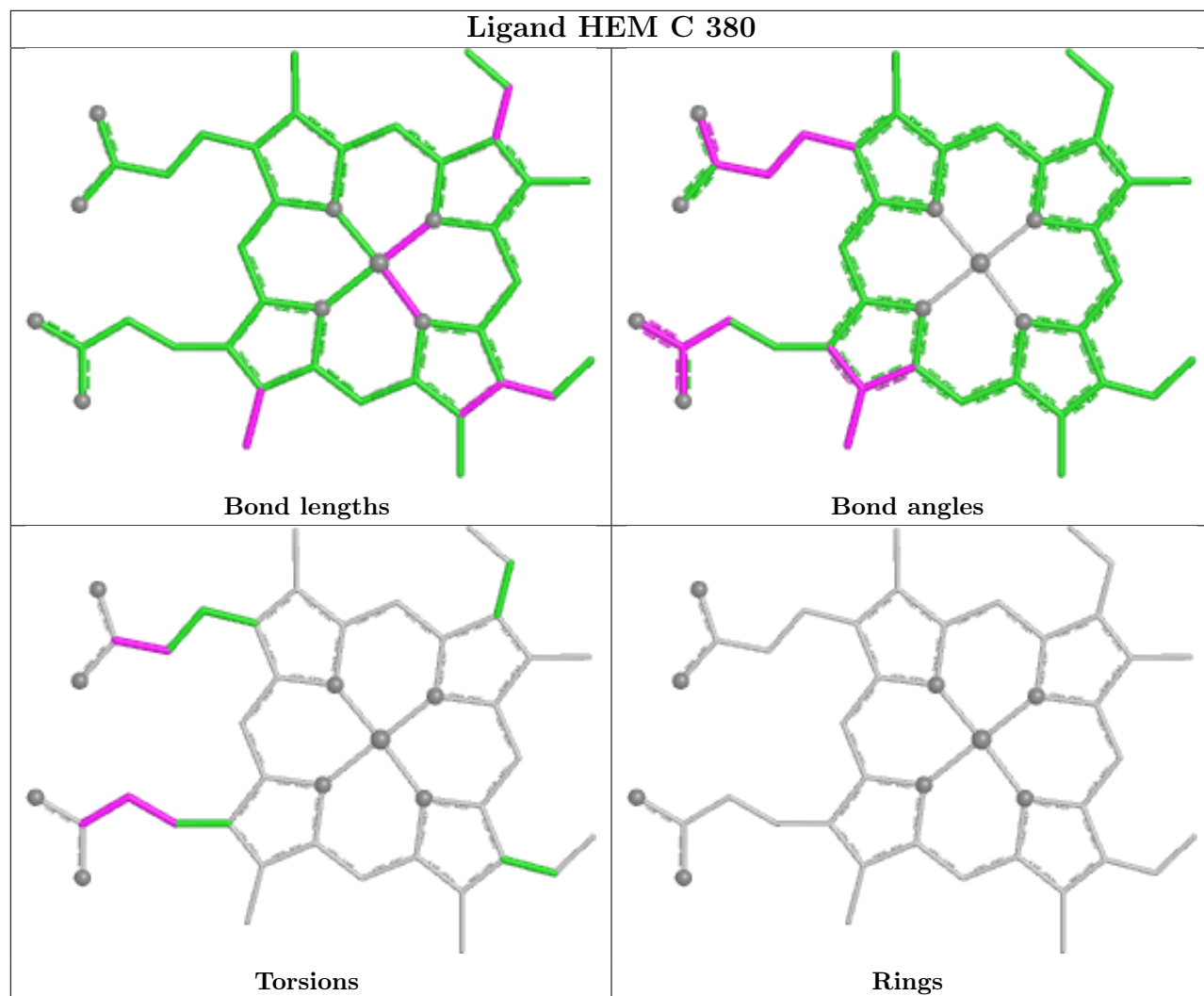
Mol	Chain	Res	Type	Atoms
13	D	242	HEC	C2B-C3B-CAB-CBB
13	D	242	HEC	C4B-C3B-CAB-CBB
13	D	242	HEC	C1A-C2A-CAA-CBA
13	D	242	HEC	C3A-C2A-CAA-CBA
13	D	242	HEC	C2A-CAA-CBA-CGA

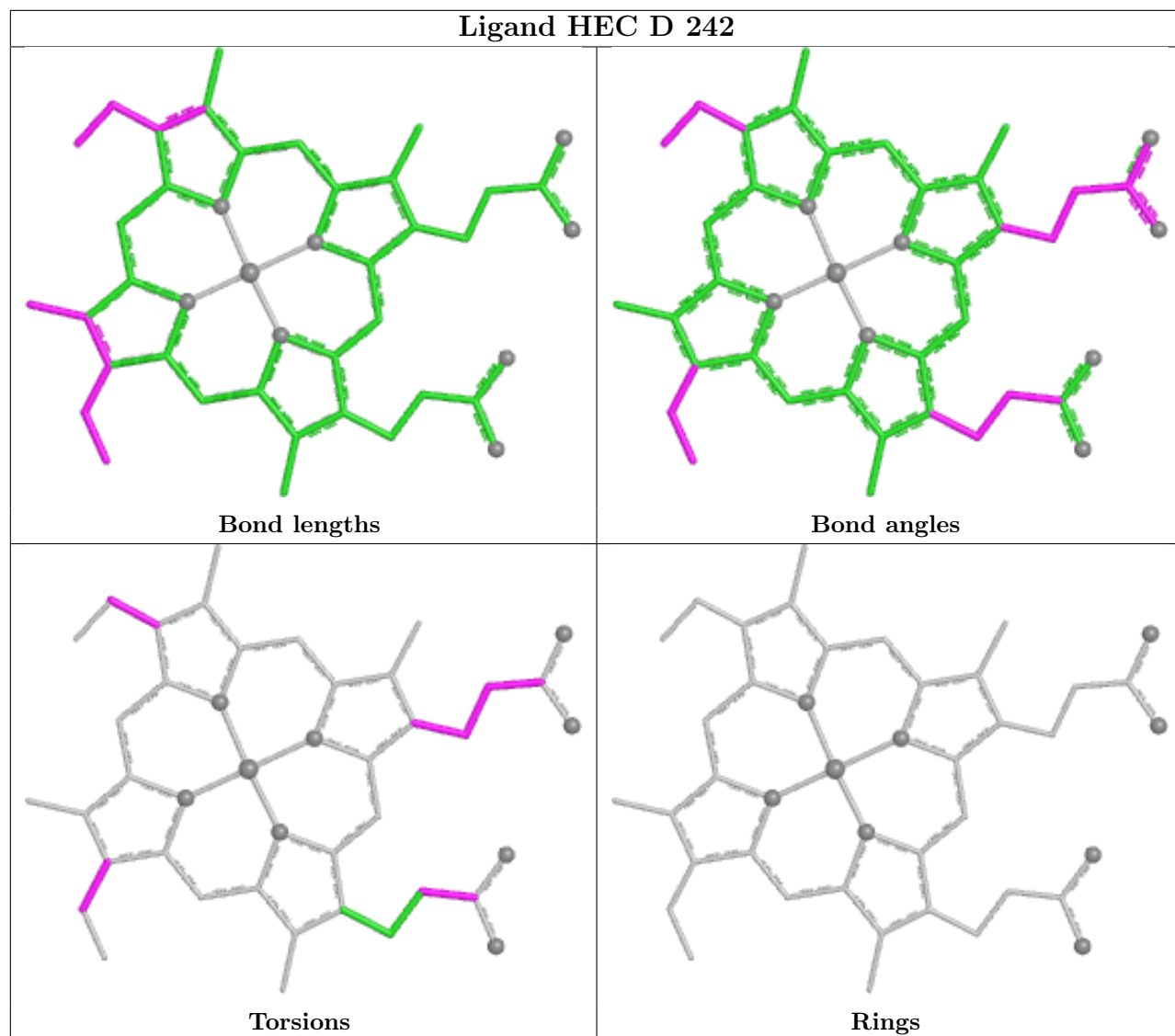
There are no ring outliers.

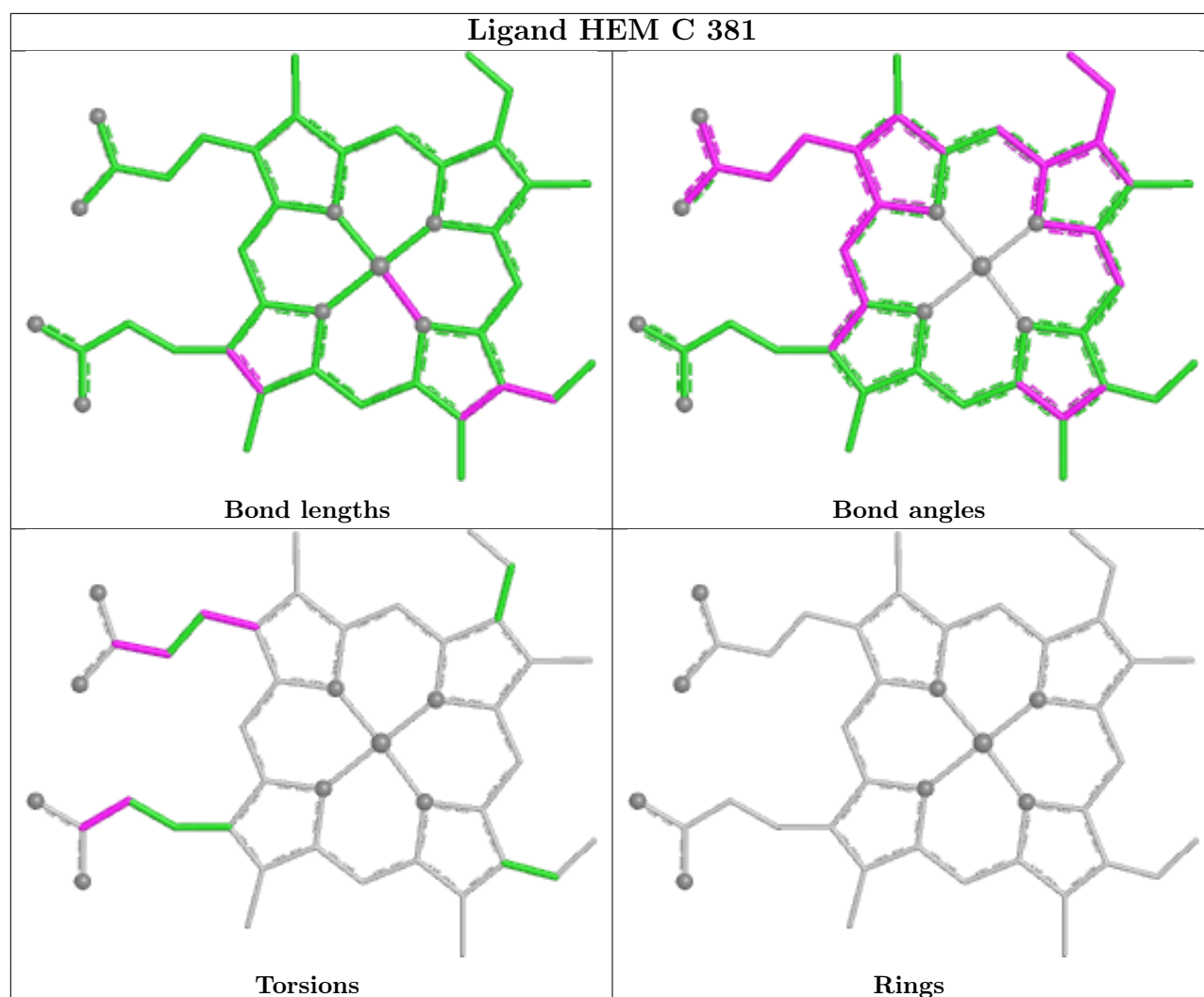
4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	380	HEM	10	0
13	D	242	HEC	3	0
12	C	381	HEM	9	0
14	E	197	FES	1	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.







## 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.