



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 11, 2024 – 01:08 AM EST

PDB ID : 1NEK
Title : Complex II (Succinate Dehydrogenase) From E. Coli with ubiquinone bound
Authors : Yankovskaya, V.; Horsefield, R.; Tornroth, S.; Luna-Chavez, C.; Miyoshi, H.;
Leger, C.; Byrne, B.; Cecchini, G.; Iwata, S.
Deposited on : 2002-12-11
Resolution : 2.60 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

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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

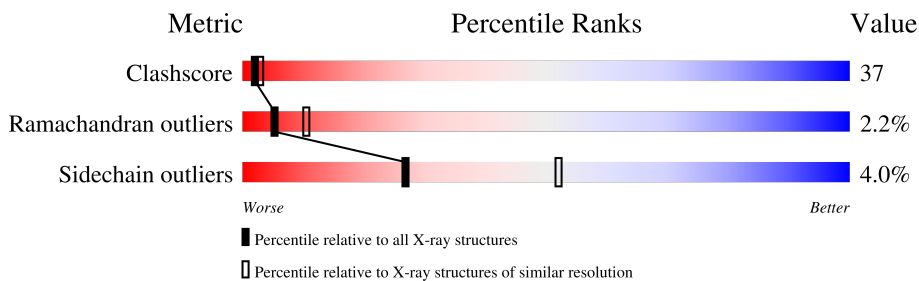
1 Overall quality at a glance

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	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (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	588	38% 57% 5%
2	B	238	54% 44% .
3	C	129	70% 29% .
4	D	115	63% 35% ..

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
10	F3S	B	304	-	-	X	-
12	CDN	C	308	X	-	-	-
8	FES	B	302	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 8698 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 Succinate dehydrogenase flavoprotein subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	89	0	0
			4522	2812	821	861	28			

- Molecule 2 is a protein called Succinate dehydrogenase iron-sulfur protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	238	Total	C	N	O	S	0	0	0
			1869	1172	329	348	20			

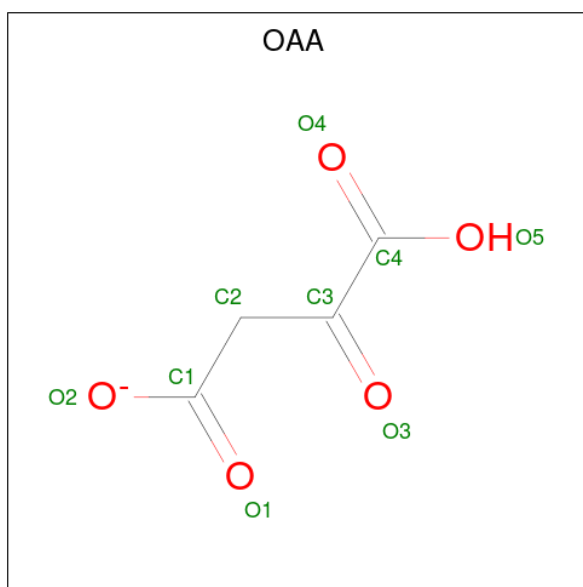
- Molecule 3 is a protein called Succinate dehydrogenase cytochrome b-556 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	129	Total	C	N	O	S	0	0	0
			1008	668	166	168	6			

- Molecule 4 is a protein called Succinate dehydrogenase hydrophobic membrane anchor protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	113	Total	C	N	O	S	0	0	0
			898	615	136	144	3			

- Molecule 5 is OXALOACETATE ION (three-letter code: OAA) (formula: C₄H₃O₅).

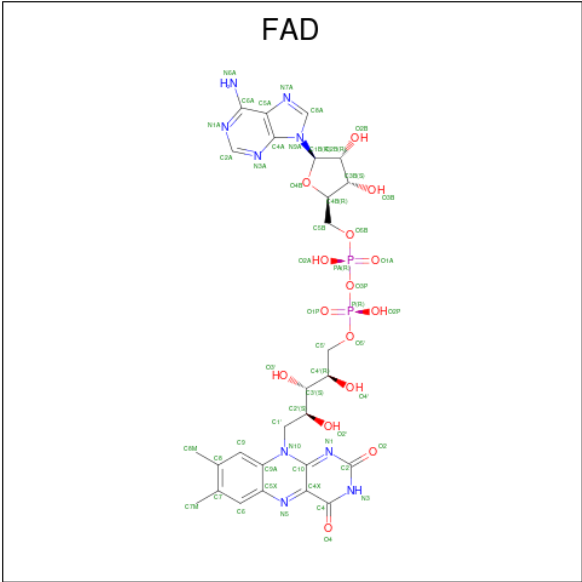


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			9	4	5		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

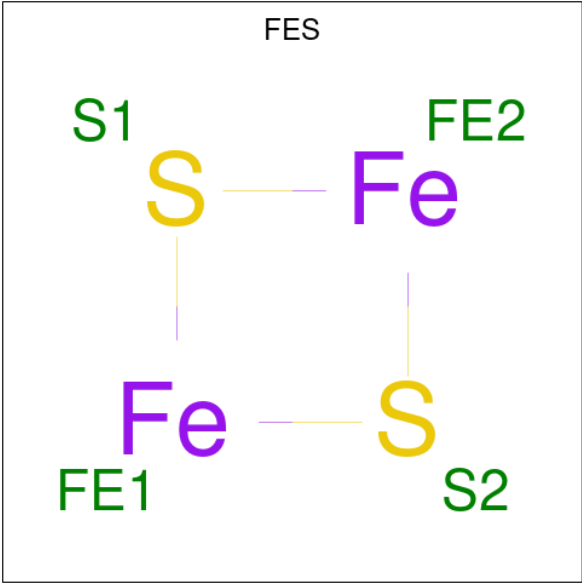
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		
6	B	1	Total	Ca	0	0
			1	1		

- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



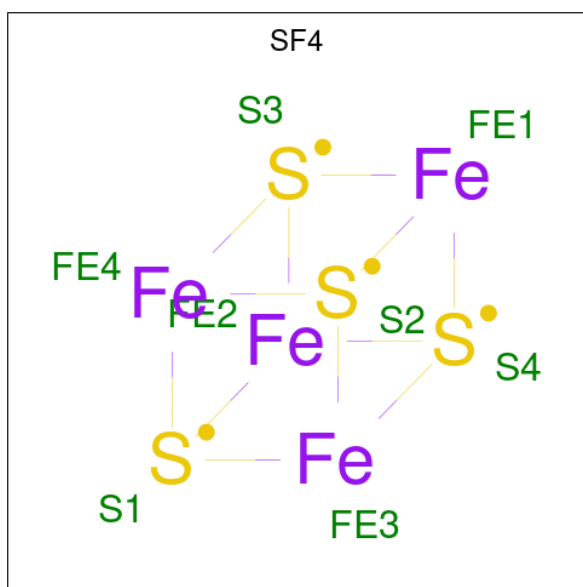
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 8 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



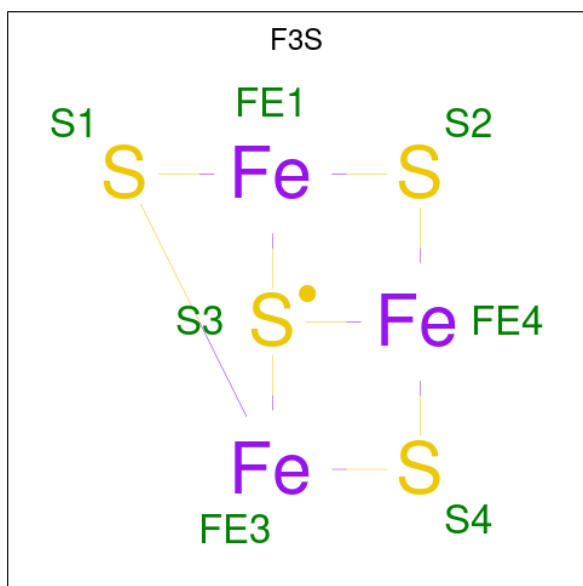
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 9 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



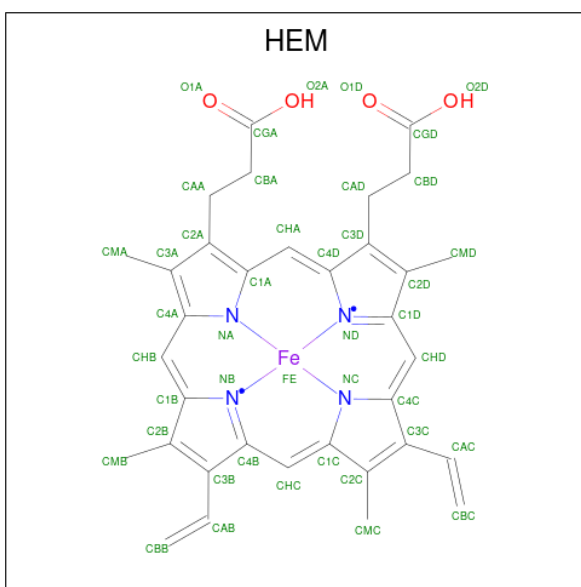
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 10 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



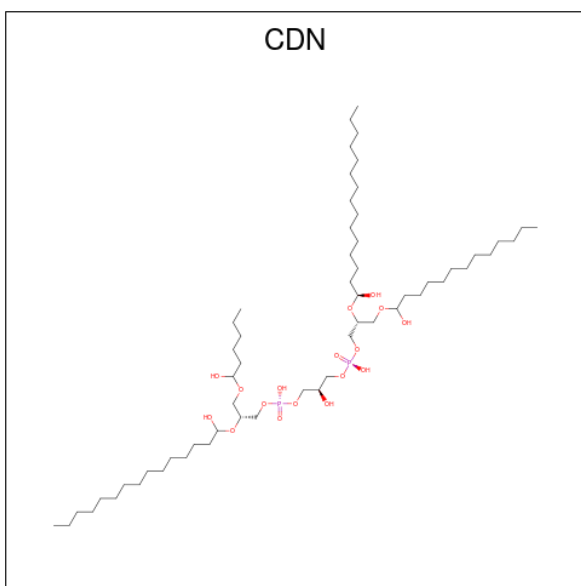
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



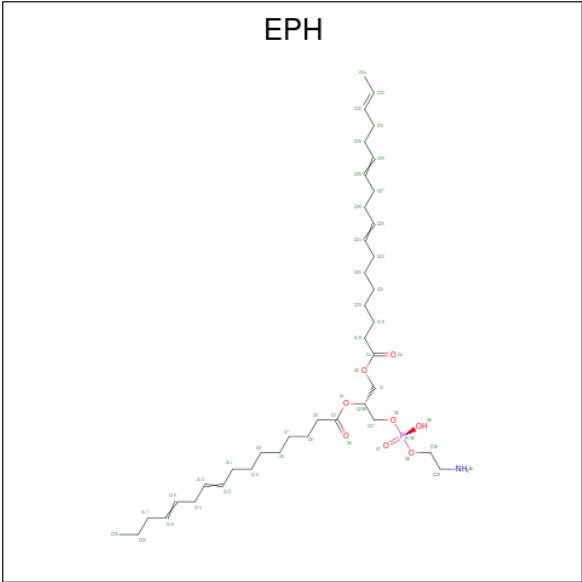
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
							0	0

- Molecule 12 is CARDIOLIPIN (three-letter code: CDN) (formula: $C_{58}H_{120}O_{17}P_2$).



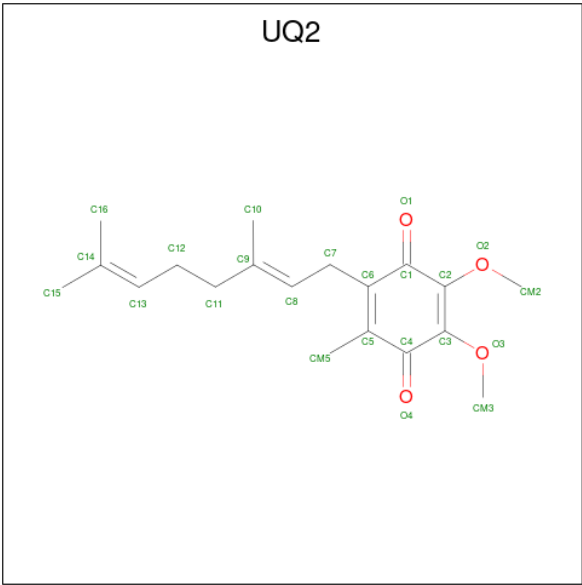
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	1	Total	C	O	P		
			77	58	17	2		
							0	0

- Molecule 13 is L-ALPHA-PHOSPHATIDYL-BETA-OLEOYL-GAMMA-PALMITOYL-PHOSPHATIDYLETHANOLAMINE (three-letter code: EPH) (formula: $C_{39}H_{68}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	N	O	P	0	0
			35	25	1	8	1		

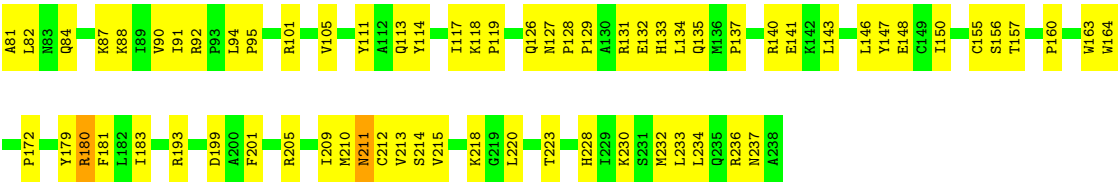
- Molecule 14 is UBIQUINONE-2 (three-letter code: UQ2) (formula: C₁₉H₂₆O₄).



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

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	61	Total 61	O 61	0	0
15	B	50	Total 50	O 50	0	0
15	C	15	Total 15	O 15	0	0
15	D	14	Total 14	O 14	0	0



● Molecule 3: Succinate dehydrogenase cytochrome b-556 subunit



● Molecule 4: Succinate dehydrogenase hydrophobic membrane anchor protein



4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	138.80Å 138.80Å 521.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.247 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8698	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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: SF4, HEM, UQ2, EPH, FAD, F3S, CA, FES, OAA, CDN

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	0.36	0/4611	0.66	1/6237 (0.0%)
2	B	0.40	0/1908	0.64	0/2578
3	C	0.41	0/1030	0.63	0/1394
4	D	0.44	0/923	0.62	0/1262
All	All	0.38	0/8472	0.65	1/11471 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	GLY	N-CA-C	-5.09	100.37	113.10

There are no chirality outliers.

There are no planarity outliers.

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	4522	0	4426	445	0
2	B	1869	0	1850	131	0
3	C	1008	0	1066	40	0
4	D	898	0	936	41	0
5	A	9	0	2	3	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
7	A	53	0	29	8	0
8	B	4	0	0	2	0
9	B	8	0	0	1	0
10	B	7	0	0	3	0
11	C	43	0	30	5	0
12	C	77	0	112	5	0
13	C	35	0	40	1	0
14	D	23	0	26	4	0
15	A	61	0	0	4	0
15	B	50	0	0	0	0
15	C	15	0	0	1	0
15	D	14	0	0	0	0
All	All	8698	0	8517	626	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 37.

The worst 5 of 626 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:559:TYR:HB2	1:A:569:ARG:NH2	1.66	1.09
3:C:6:LYS:HG2	3:C:7:LYS:H	1.19	1.06
1:A:584:LYS:HG2	1:A:585:ILE:H	1.19	1.05
1:A:534:THR:HB	1:A:553:TRP:HE1	1.21	1.04
2:B:95:PRO:HD2	2:B:157:THR:HG22	1.38	1.04

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	586/588 (100%)	504 (86%)	65 (11%)	17 (3%)	3	6
2	B	236/238 (99%)	205 (87%)	28 (12%)	3 (1%)	10	21
3	C	127/129 (98%)	117 (92%)	7 (6%)	3 (2%)	5	9
4	D	111/115 (96%)	107 (96%)	4 (4%)	0	100	100
All	All	1060/1070 (99%)	933 (88%)	104 (10%)	23 (2%)	5	10

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	GLY
1	A	110	ASP
1	A	119	PHE
1	A	278	PRO
3	C	7	LYS

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	473/473 (100%)	448 (95%)	25 (5%)	19	40
2	B	208/208 (100%)	203 (98%)	5 (2%)	44	70
3	C	109/109 (100%)	107 (98%)	2 (2%)	54	77
4	D	94/96 (98%)	91 (97%)	3 (3%)	34	60
All	All	884/886 (100%)	849 (96%)	35 (4%)	27	52

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	180	ARG
2	B	211	ASN
4	D	6	SER
1	A	436	ASP
1	A	384	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	470	ASN
4	D	94	GLN
1	A	572	ASN
3	C	30	HIS
1	A	540	HIS

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](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 for Mogul analysis.

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	$\# Z > 2$
11	HEM	C	305	4,3	42,50,50	1.52	6 (14%)	46,82,82	2.02	13 (28%)
12	CDN	C	308	-	76,76,76	2.05	11 (14%)	74,88,88	1.65	9 (12%)
8	FES	B	302	2	0,4,4	-	-	-	-	-
13	EPH	C	309	-	34,34,48	1.13	3 (8%)	37,39,53	0.96	2 (5%)
5	OAA	A	589	-	8,8,8	4.68	3 (37%)	8,10,10	2.32	4 (50%)
7	FAD	A	601	1	54,58,58	2.29	16 (29%)	71,89,89	1.23	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	UQ2	D	306	-	23,23,23	2.74	9 (39%)	30,31,31	1.39	3 (10%)
9	SF4	B	303	2	0,12,12	-	-	-		
10	F3S	B	304	2	0,9,9	-	-	-		

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
11	HEM	C	305	4,3	-	6/12/54/54	-
12	CDN	C	308	-	3/3/9/9	24/87/87/87	-
8	FES	B	302	2	-	-	0/1/1/1
13	EPH	C	309	-	-	6/38/38/52	-
5	OAA	A	589	-	-	2/8/8/8	-
7	FAD	A	601	1	-	3/30/50/50	0/6/6/6
14	UQ2	D	306	-	-	4/15/39/39	0/1/1/1
9	SF4	B	303	2	-	-	0/6/5/5
10	F3S	B	304	2	-	-	0/3/3/3

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	589	OAA	C3-C4	-12.51	1.34	1.53
14	D	306	UQ2	C7-C8	-10.03	1.34	1.50
7	A	601	FAD	C4X-N5	7.54	1.47	1.30
12	C	308	CDN	OA8-CA7	7.41	1.53	1.40
12	C	308	CDN	OA6-CA5	-7.12	1.21	1.41

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	308	CDN	OB9-CB7-C71	5.81	125.22	109.37
12	C	308	CDN	OB7-CB5-C51	5.67	124.84	109.37
12	C	308	CDN	OA9-CA7-C31	5.65	124.80	109.37
11	C	305	HEM	CHC-C4B-NB	4.85	129.65	124.44
5	A	589	OAA	O3-C3-C2	4.57	127.44	120.41

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	C	308	CDN	CA7
12	C	308	CDN	CB5
12	C	308	CDN	CB7

5 of 45 torsion outliers are listed below:

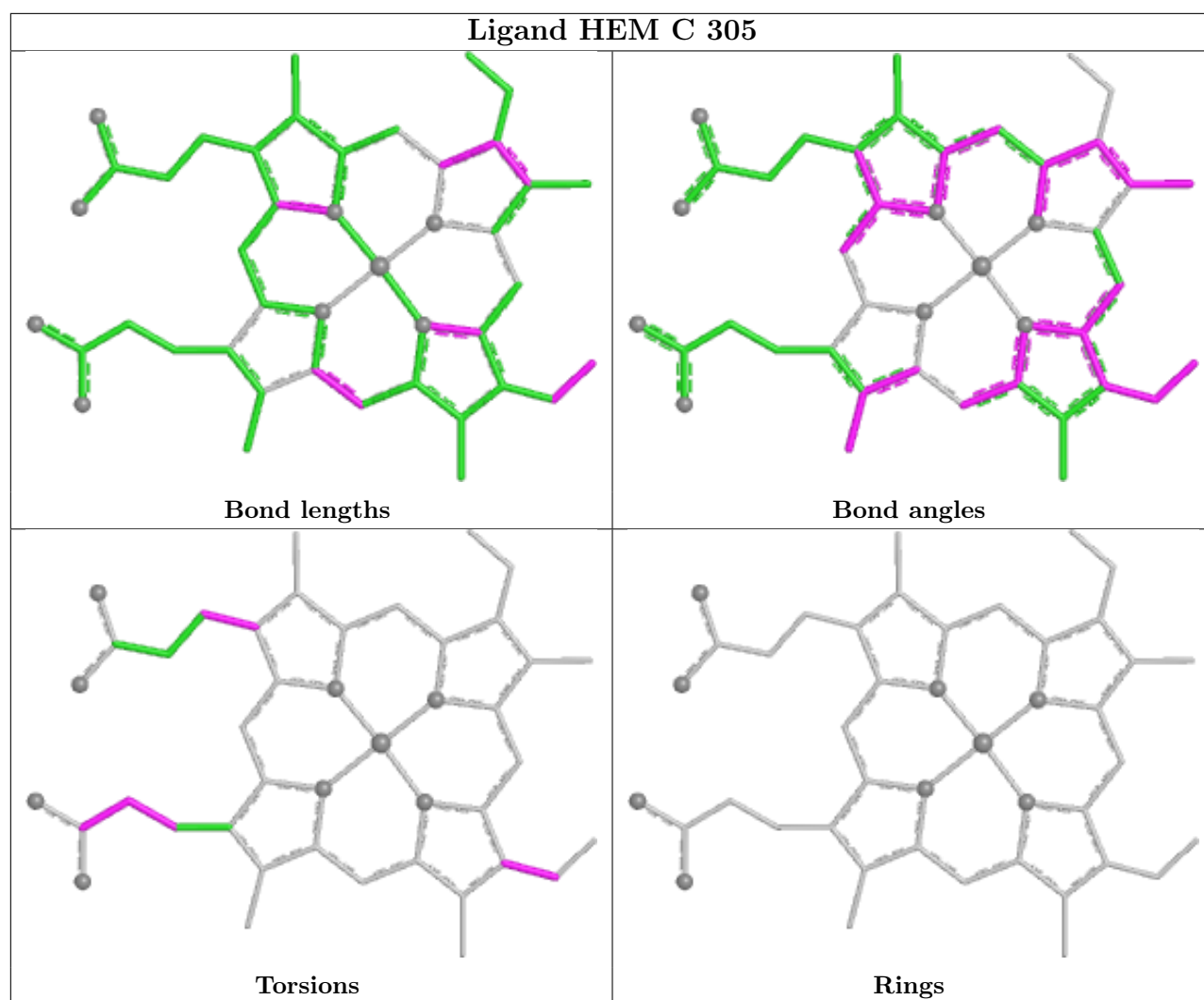
Mol	Chain	Res	Type	Atoms
11	C	305	HEM	C2B-C3B-CAB-CBB
11	C	305	HEM	C4B-C3B-CAB-CBB
12	C	308	CDN	CB2-OB2-PB2-OB5
12	C	308	CDN	CB2-OB2-PB2-OB3
12	C	308	CDN	CB2-OB2-PB2-OB4

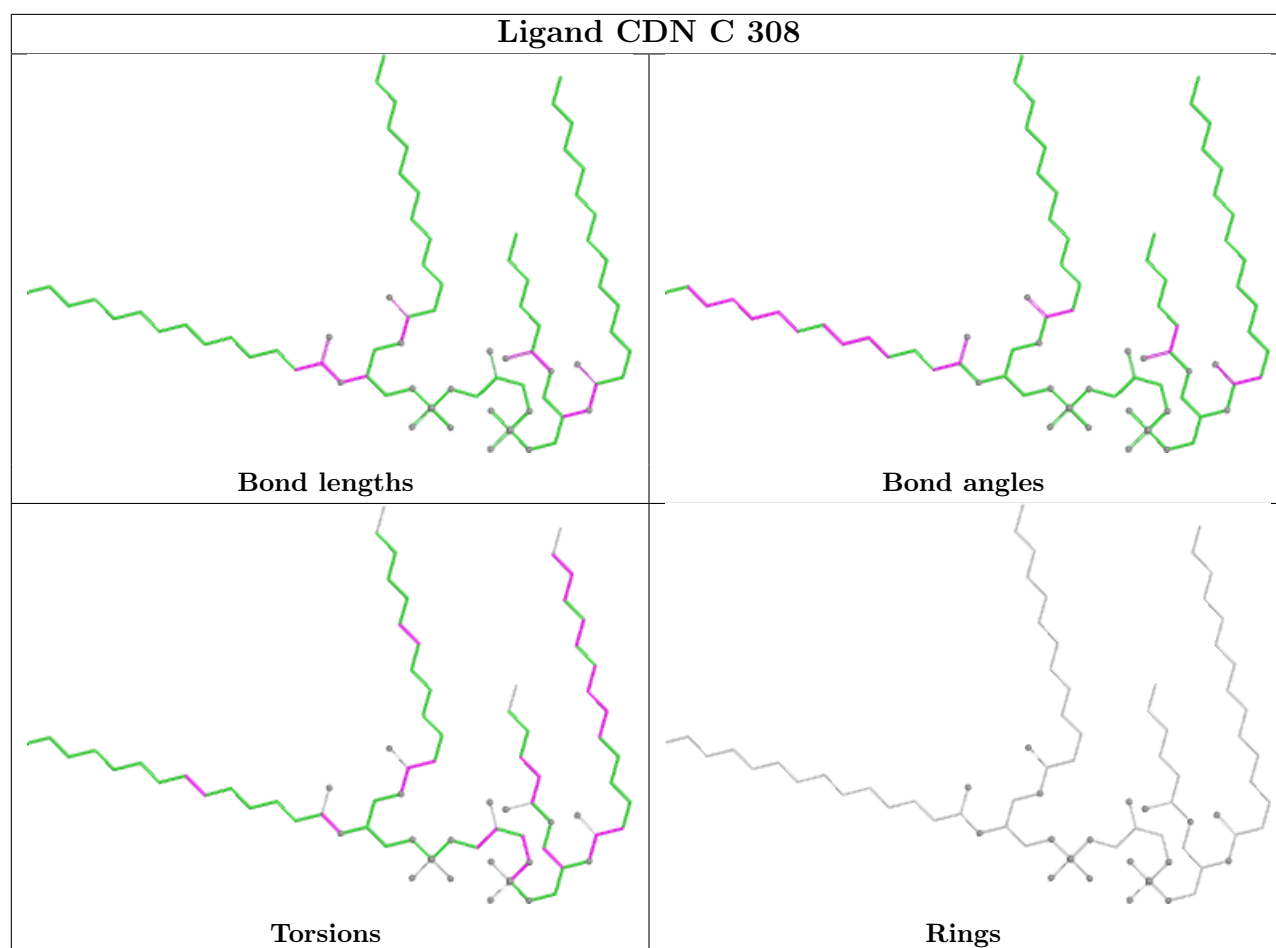
There are no ring outliers.

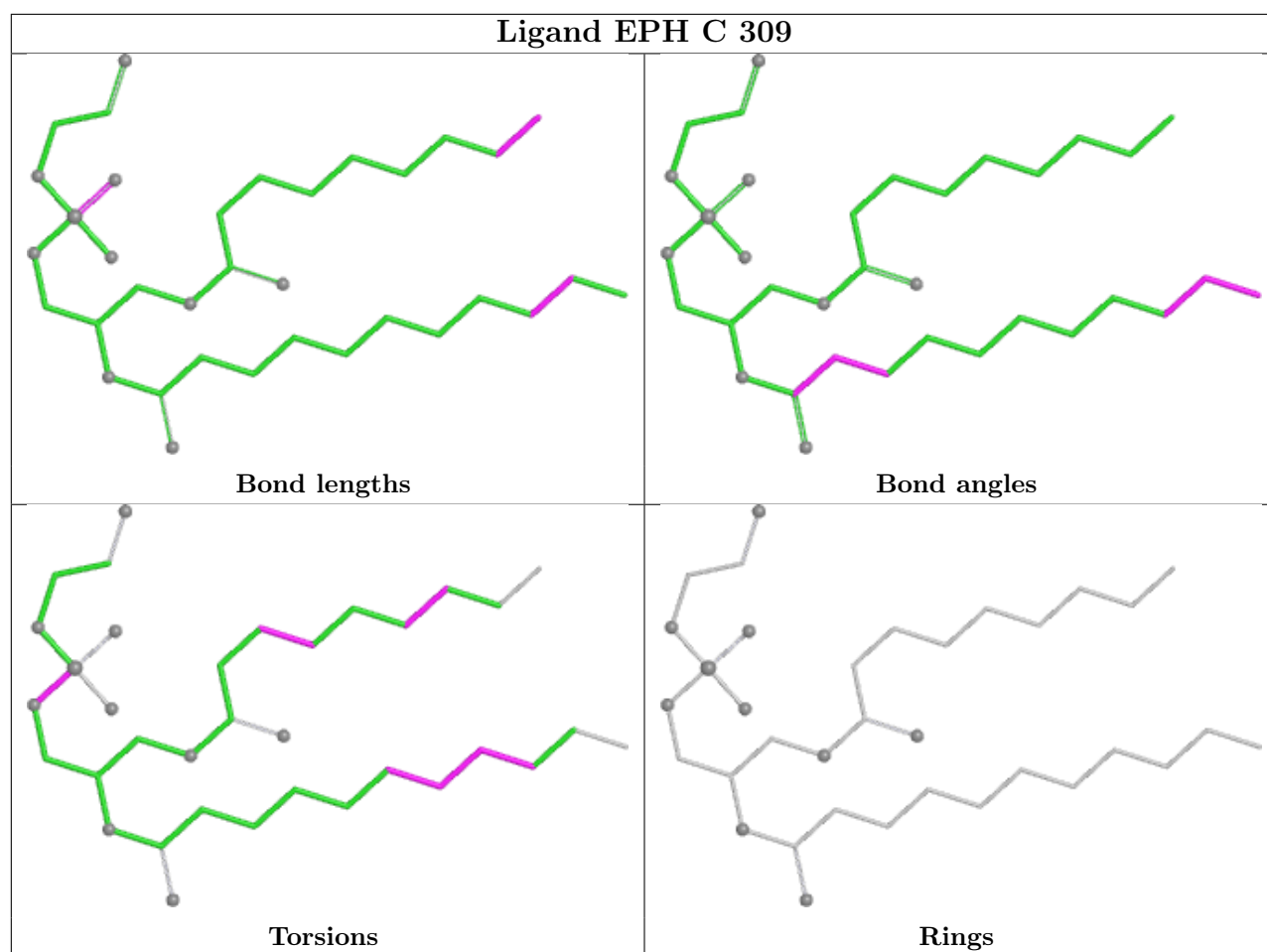
9 monomers are involved in 31 short contacts:

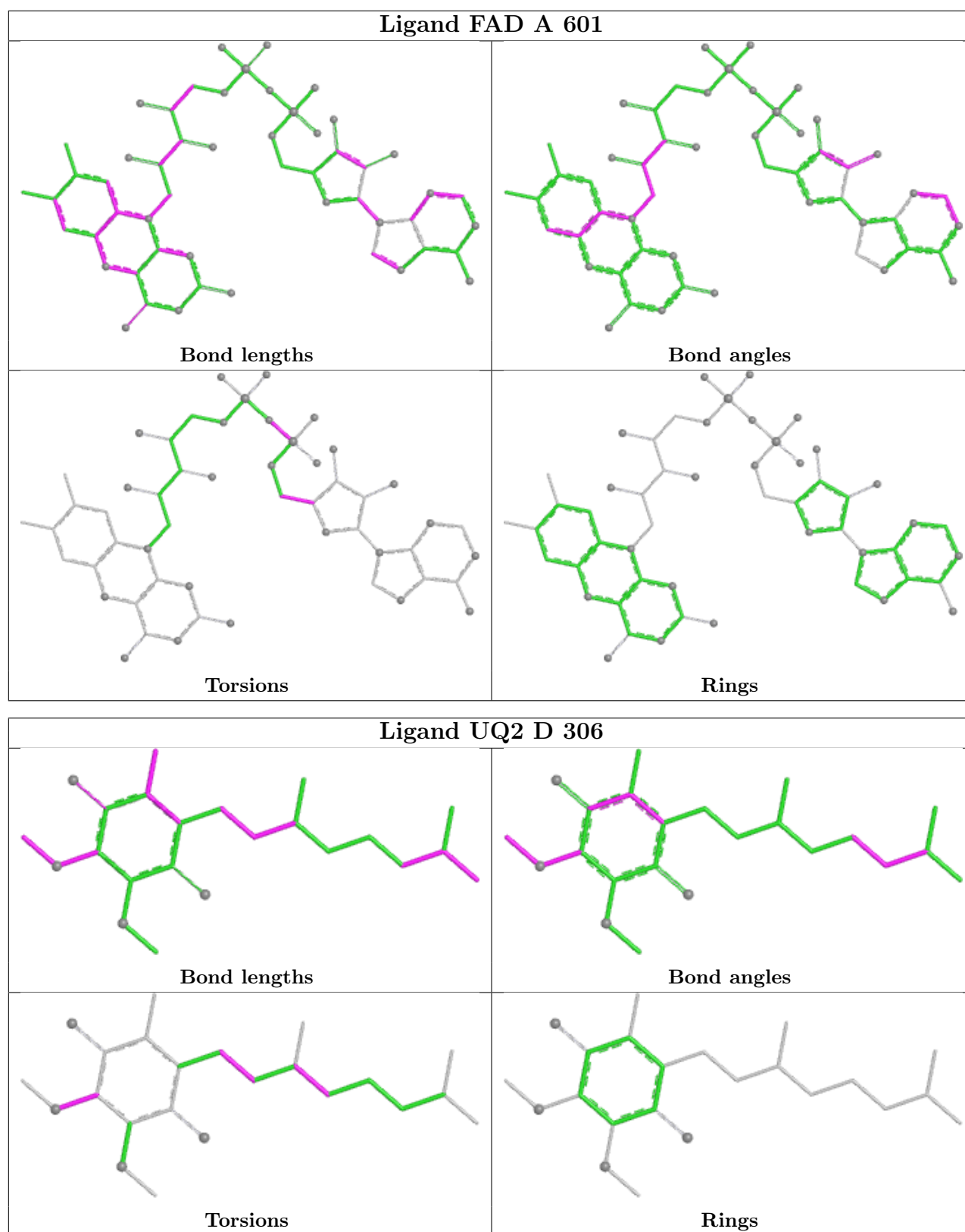
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	305	HEM	5	0
12	C	308	CDN	5	0
8	B	302	FES	2	0
13	C	309	EPH	1	0
5	A	589	OAA	3	0
7	A	601	FAD	8	0
14	D	306	UQ2	4	0
9	B	303	SF4	1	0
10	B	304	F3S	3	0

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 ⓘ

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.