



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 08:34 AM EDT

PDB ID : 1ESZ
Title : STRUCTURE OF THE PERIPLASMIC FERRIC SIDEROPHORE BINDING PROTEIN FHUD COMPLEXED WITH COPROGEN
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Deposited on : 2000-04-11
Resolution : 2.00 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

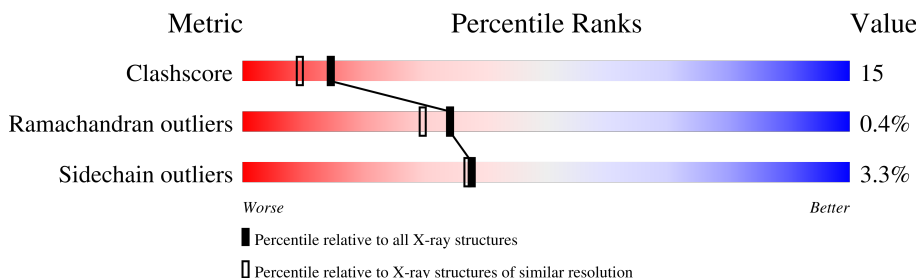
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 ≥ 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	266	72% 24% ..

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
2	CPO	A	500	X	-	-	-

2 Entry composition [i](#)

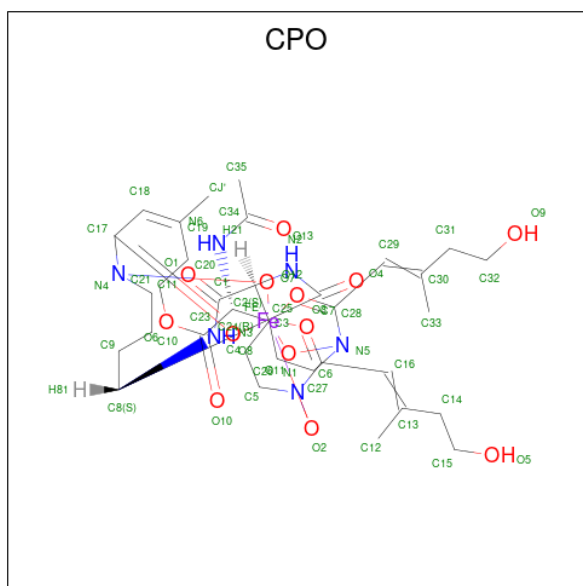
There are 3 unique types of molecules in this entry. The entry contains 2200 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FERRICHRONE-BINDING PERIPLASMIC PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			2021	1309	336	364	12			

- Molecule 2 is COPROGEN (three-letter code: CPO) (formula: $C_{35}H_{53}FeN_6O_{13}$).

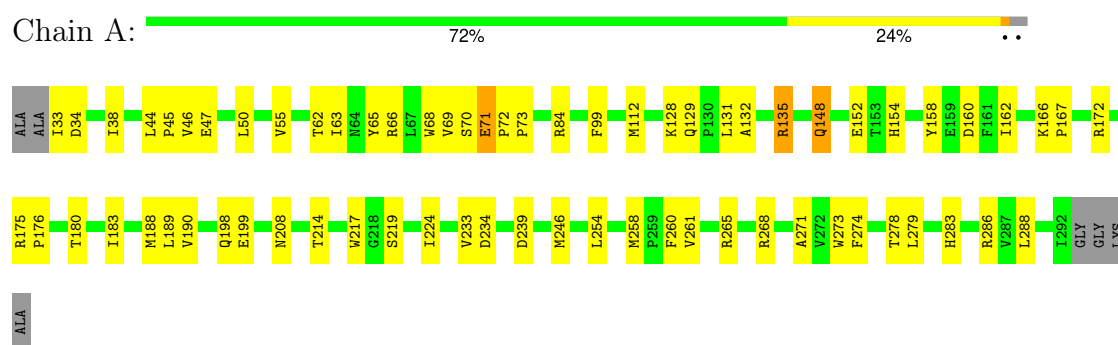


3 Residue-property plots

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: FERRICHROME-BINDING PERIPLASMIC PROTEIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	86.09Å 86.09Å 91.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.00	Depositor
% Data completeness (in resolution range)	95.6 (30.00-2.00)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2200	wwPDB-VP
Average B, all atoms (Å ²)	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: CPO

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	0.34	0/2078	0.59	0/2841

There are no bond length outliers.

There are no bond angle outliers.

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	2021	0	1972	62	1
2	A	54	0	49	5	0
3	A	125	0	0	3	0
All	All	2200	0	2021	63	1

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 15.

All (63) 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:132:ALA:HA	1:A:135:ARG:HH12	1.15	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ILE:HD12	1:A:63:ILE:H	1.26	0.98
1:A:71:GLU:HB3	1:A:72:PRO:HD3	1.48	0.95
1:A:183:ILE:HD11	1:A:189:LEU:HG	1.56	0.86
1:A:132:ALA:HA	1:A:135:ARG:NH1	1.93	0.84
1:A:224:ILE:H	1:A:224:ILE:HD12	1.44	0.83
1:A:176:PRO:HG2	1:A:233:VAL:HG12	1.67	0.73
1:A:84:ARG:HD3	3:A:690:HOH:O	1.87	0.73
1:A:55:VAL:HG22	3:A:651:HOH:O	1.93	0.69
1:A:148:GLN:NE2	1:A:148:GLN:H	1.91	0.68
1:A:63:ILE:H	1:A:63:ILE:CD1	2.01	0.68
1:A:71:GLU:HG2	1:A:286:ARG:HH21	1.59	0.67
1:A:148:GLN:H	1:A:148:GLN:HE21	1.42	0.66
1:A:224:ILE:HD12	1:A:224:ILE:N	2.10	0.66
1:A:71:GLU:HG2	1:A:286:ARG:NH2	2.12	0.64
1:A:71:GLU:HB3	1:A:72:PRO:CD	2.25	0.64
1:A:62:THR:O	1:A:66:ARG:HG3	1.98	0.63
1:A:46:VAL:O	1:A:50:LEU:HD13	1.99	0.62
1:A:224:ILE:H	1:A:224:ILE:CD1	2.12	0.62
1:A:69:VAL:HG12	1:A:72:PRO:HD2	1.82	0.61
1:A:38:ILE:HD12	1:A:99:PHE:HB3	1.82	0.61
1:A:183:ILE:HD13	2:A:500:CPO:H353	1.84	0.60
1:A:166:LYS:N	1:A:167:PRO:HD2	2.18	0.59
1:A:198:GLN:HE22	1:A:208:ASN:HB2	1.67	0.59
1:A:239:ASP:OD1	1:A:268:ARG:HD2	2.03	0.59
1:A:63:ILE:HD12	1:A:63:ILE:N	2.08	0.58
1:A:217:TRP:CH2	2:A:500:CPO:H32	2.38	0.58
1:A:189:LEU:HD22	1:A:219:SER:HB2	1.85	0.58
1:A:217:TRP:CZ3	2:A:500:CPO:H32	2.39	0.58
1:A:158:TYR:O	1:A:162:ILE:HG12	2.05	0.57
1:A:198:GLN:NE2	1:A:208:ASN:HD22	2.03	0.57
1:A:71:GLU:HB2	1:A:283:HIS:CD2	2.39	0.57
1:A:258:MET:HG2	1:A:260:PHE:CZ	2.40	0.55
1:A:33:ILE:HG23	1:A:34:ASP:N	2.22	0.54
1:A:71:GLU:O	1:A:73:PRO:HD3	2.08	0.53
1:A:175:ARG:HB2	1:A:175:ARG:NH1	2.23	0.53
1:A:47:GLU:OE1	1:A:279:LEU:N	2.42	0.52
1:A:234:ASP:OD1	1:A:265:ARG:HD2	2.09	0.52
1:A:131:LEU:HD12	1:A:199:GLU:HB3	1.90	0.52
1:A:154:HIS:HE1	1:A:278:THR:OG1	1.91	0.51
1:A:65:TYR:OH	1:A:72:PRO:HB2	2.10	0.50
1:A:172:ARG:HD3	3:A:665:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLU:CG	1:A:286:ARG:HH21	2.26	0.49
1:A:128:LYS:HG2	1:A:129:GLN:HG3	1.95	0.48
1:A:175:ARG:HB2	1:A:175:ARG:HH11	1.78	0.47
1:A:239:ASP:O	1:A:271:ALA:HB2	2.15	0.46
1:A:246:MET:HE3	1:A:268:ARG:HD3	1.99	0.45
1:A:68:TRP:NE1	2:A:500:CPO:H311	2.32	0.45
1:A:55:VAL:HG23	1:A:55:VAL:O	2.16	0.44
1:A:198:GLN:HE22	1:A:208:ASN:HD22	1.65	0.44
1:A:246:MET:CE	1:A:268:ARG:HD3	2.47	0.44
2:A:500:CPO:H161	2:A:500:CPO:H51	1.81	0.44
1:A:33:ILE:CG2	1:A:34:ASP:N	2.81	0.43
1:A:273:TRP:HA	1:A:273:TRP:CE3	2.54	0.43
1:A:172:ARG:NH2	1:A:234:ASP:OD2	2.47	0.42
1:A:135:ARG:HB2	1:A:135:ARG:HH11	1.83	0.42
1:A:180:THR:HG22	1:A:190:VAL:HG22	2.03	0.41
1:A:44:LEU:HB3	1:A:45:PRO:CD	2.50	0.41
1:A:47:GLU:HG3	1:A:279:LEU:HD12	2.03	0.41
1:A:112:MET:SD	1:A:112:MET:C	2.99	0.40
1:A:148:GLN:O	1:A:152:GLU:HG3	2.21	0.40
1:A:198:GLN:HE22	1:A:208:ASN:CB	2.31	0.40
1:A:258:MET:HB3	1:A:261:VAL:CG2	2.51	0.40

All (1) 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)
1:A:160:ASP:OD2	1:A:214:THR:O[2_545]	2.19	0.01

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	258/266 (97%)	248 (96%)	9 (4%)	1 (0%)	34 30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	SER

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	211/221 (96%)	204 (97%)	7 (3%)	38 37

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	135	ARG
1	A	148	GLN
1	A	188	MET
1	A	254	LEU
1	A	274	PHE
1	A	288	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	148	GLN
1	A	154	HIS
1	A	198	GLN
1	A	240	HIS
1	A	283	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
2	CPO	A	500	-	54,59,60	3.13	20 (37%)	51,89,91	2.45	24 (47%)

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
2	CPO	A	500	-	3/3/16/23	20/48/118/120	0/3/6/6

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	CPO	C29-C30	12.27	1.55	1.33
2	A	500	CPO	C18-C17	8.21	1.57	1.46
2	A	500	CPO	C16-C13	7.47	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	CPO	O6-C23	6.27	1.46	1.33
2	A	500	CPO	C27-N5	-4.77	1.38	1.47
2	A	500	CPO	C31-C30	4.35	1.60	1.51
2	A	500	CPO	O7-N4	-4.19	1.31	1.38
2	A	500	CPO	O3-C6	-3.86	1.20	1.28
2	A	500	CPO	C24-N6	-3.75	1.38	1.45
2	A	500	CPO	C1-N3	3.33	1.38	1.33
2	A	500	CPO	C8-N3	-3.32	1.41	1.46
2	A	500	CPO	C8-C7	3.23	1.59	1.52
2	A	500	CPO	C12-C13	3.21	1.58	1.50
2	A	500	CPO	C2-N2	-2.90	1.42	1.46
2	A	500	CPO	C7-N2	2.83	1.37	1.33
2	A	500	CPO	O12-C28	-2.72	1.23	1.28
2	A	500	CPO	O13-C34	2.67	1.29	1.23
2	A	500	CPO	C14-C13	2.62	1.56	1.51
2	A	500	CPO	C33-C30	-2.41	1.44	1.50
2	A	500	CPO	C3-C2	2.06	1.58	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	CPO	C9-C8-N3	-5.32	100.36	110.97
2	A	500	CPO	C9-C8-C7	-5.11	97.36	111.10
2	A	500	CPO	C10-C11-N4	4.87	120.91	110.94
2	A	500	CPO	C26-C27-N5	4.76	120.69	110.94
2	A	500	CPO	C3-C2-N2	-4.24	102.50	110.97
2	A	500	CPO	C25-C24-N6	-3.89	103.22	110.91
2	A	500	CPO	C21-O6-C23	-3.80	108.18	116.53
2	A	500	CPO	O11-N5-C27	3.69	120.29	114.13
2	A	500	CPO	O2-N1-C5	3.64	120.22	114.13
2	A	500	CPO	O7-N4-C11	3.59	120.13	114.13
2	A	500	CPO	O6-C23-C24	3.56	119.94	111.58
2	A	500	CPO	C4-C3-C2	3.09	123.32	113.80
2	A	500	CPO	C24-N6-C34	3.09	130.25	121.58
2	A	500	CPO	C20-C19-C18	-2.85	119.98	125.92
2	A	500	CPO	C10-C9-C8	2.85	122.57	113.80
2	A	500	CPO	C12-C13-C14	2.69	119.90	115.23
2	A	500	CPO	C23-C24-N6	-2.65	104.53	110.65
2	A	500	CPO	C35-C34-N6	2.43	120.14	116.12
2	A	500	CPO	O1-C1-N3	-2.37	119.54	122.67
2	A	500	CPO	C33-C30-C29	-2.29	116.15	122.90
2	A	500	CPO	O6-C23-O10	-2.26	120.01	124.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	CPO	C31-C30-C29	-2.14	115.72	121.90
2	A	500	CPO	C3-C4-C5	2.04	119.31	113.29
2	A	500	CPO	C19-C18-C17	2.00	126.15	123.23

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	500	CPO	N1
2	A	500	CPO	N4
2	A	500	CPO	N5

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	CPO	C1-C2-C3-C4
2	A	500	CPO	N2-C2-C3-C4
2	A	500	CPO	C3-C4-C5-N1
2	A	500	CPO	C9-C10-C11-N4
2	A	500	CPO	C12-C13-C16-C6
2	A	500	CPO	C14-C13-C16-C6
2	A	500	CPO	N4-C17-C18-C19
2	A	500	CPO	O8-C17-C18-C19
2	A	500	CPO	C17-C18-C19-C20
2	A	500	CPO	C30-C31-C32-O9
2	A	500	CPO	O13-C34-N6-C24
2	A	500	CPO	C35-C34-N6-C24
2	A	500	CPO	C29-C30-C31-C32
2	A	500	CPO	O10-C23-O6-C21
2	A	500	CPO	C24-C23-O6-C21
2	A	500	CPO	C28-C29-C30-C31
2	A	500	CPO	C7-C8-C9-C10
2	A	500	CPO	C24-C25-C26-C27
2	A	500	CPO	O10-C23-C24-C25
2	A	500	CPO	O6-C23-C24-C25

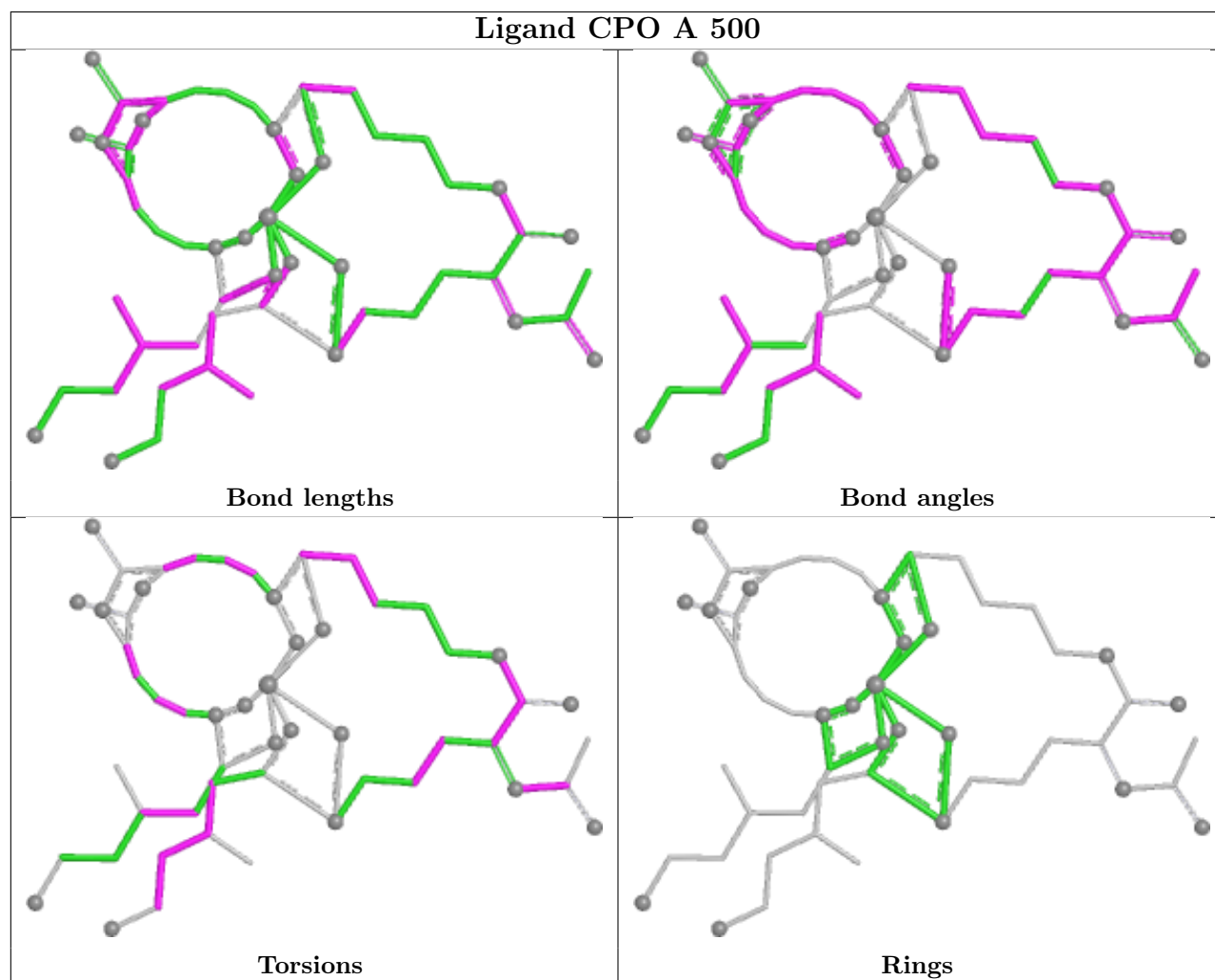
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	CPO	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.



5.7 Other polymers ⓘ

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.