# wwPDB EM Validation Summary Report

May 2, 2024 – 06:08 PM JST

| | | |
|---|---|---|
| PDB ID | : | 8JT6 |
| EMDB ID | : | EMD-36634 |
| Title | : | 5-HT1A-Gi in complex with compound (R)-IHCH-7179 |
| Authors | : | Chen, Z.; Xu, P.; Huang, S.; Xu, H.E.; Wang, S. |
| Deposited on | : | 2023-06-21 |
| Resolution | : | 3.00 Å(reported) |

This is a wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

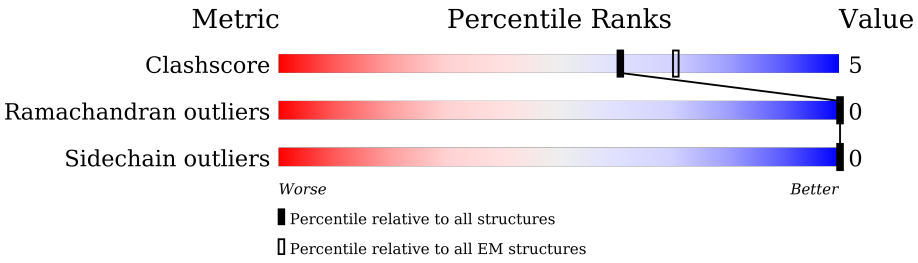
| | | |
|---|---|---|
| EMDB validation analysis | : | FAILED |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | FAILED |
| 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 (i)

The following experimental techniques were used to determine the structure:
*ELECTRON MICROSCOPY*

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) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 <=5%

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 354 | 58% · 38% |
| 2 | B | 345 | 88% 7% 5% |
| 3 | E | 269 | 82% · 14% |
| 4 | G | 67 | 66% · 33% |
| 5 | R | 544 | 46% 5% 49% |

# 2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 17718 atoms, of which 8889 are hydrogens and 0 are deuteriums.

In the tables below, 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 Guanine nucleotide-binding protein G(i) subunit alpha-1.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 1 | A | 219 | 3537 | 1126 | 1771 | 295 | 333 | 12 | 0 | 0 |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 47 | ASN | SER | conflict | UNP P63096 |
| A | 203 | ALA | GLY | conflict | UNP P63096 |
| A | 245 | ALA | GLU | conflict | UNP P63096 |
| A | 326 | SER | ALA | conflict | UNP P63096 |

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 2 | B | 328 | 4945 | 1554 | 2429 | 452 | 489 | 21 | 0 | 0 |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | -4 | MET | - | initiating methionine | UNP P62873 |
| B | -3 | GLY | - | expression tag | UNP P62873 |
| B | -2 | SER | - | expression tag | UNP P62873 |
| B | -1 | LEU | - | expression tag | UNP P62873 |
| B | 0 | LEU | - | expression tag | UNP P62873 |
| B | 1 | GLN | - | expression tag | UNP P62873 |

- Molecule 3 is a protein called ScFv16.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 3 | E | 230 | 3471 | 1120 | 1703 | 293 | 345 | 10 | 0 | 0 |

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 4 | G | 45 | Total | C | H | N | O | S | 0 | 0 |
| | | | 698 | 218 | 351 | 60 | 66 | 3 | | |

- Molecule 5 is a protein called Soluble cytochrome b562,5-hydroxytryptamine receptor 1A.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 5 | R | 278 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4497 | 1453 | 2300 | 362 | 365 | 17 | | |

There are 42 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| R | -121 | MET | - | initiating methionine | UNP P0ABE7 |
| R | -120 | ASP | - | expression tag | UNP P0ABE7 |
| R | -119 | TYR | - | expression tag | UNP P0ABE7 |
| R | -118 | LYS | - | expression tag | UNP P0ABE7 |
| R | -117 | ASP | - | expression tag | UNP P0ABE7 |
| R | -116 | ASP | - | expression tag | UNP P0ABE7 |
| R | -115 | ASP | - | expression tag | UNP P0ABE7 |
| R | -114 | ASP | - | expression tag | UNP P0ABE7 |
| R | -113 | ALA | - | expression tag | UNP P0ABE7 |
| R | -112 | LYS | - | expression tag | UNP P0ABE7 |
| R | -111 | LEU | - | expression tag | UNP P0ABE7 |
| R | -110 | GLN | - | expression tag | UNP P0ABE7 |
| R | -109 | THR | - | expression tag | UNP P0ABE7 |
| R | -108 | MET | - | expression tag | UNP P0ABE7 |
| R | -107 | HIS | - | expression tag | UNP P0ABE7 |
| R | -106 | HIS | - | expression tag | UNP P0ABE7 |
| R | -105 | HIS | - | expression tag | UNP P0ABE7 |
| R | -104 | HIS | - | expression tag | UNP P0ABE7 |
| R | -103 | HIS | - | expression tag | UNP P0ABE7 |
| R | -102 | HIS | - | expression tag | UNP P0ABE7 |
| R | -101 | HIS | - | expression tag | UNP P0ABE7 |
| R | -100 | HIS | - | expression tag | UNP P0ABE7 |
| R | -99 | HIS | - | expression tag | UNP P0ABE7 |
| R | -98 | HIS | - | expression tag | UNP P0ABE7 |
| R | -97 | HIS | - | expression tag | UNP P0ABE7 |
| R | -96 | HIS | - | expression tag | UNP P0ABE7 |
| R | -95 | HIS | - | expression tag | UNP P0ABE7 |
| R | -94 | HIS | - | expression tag | UNP P0ABE7 |

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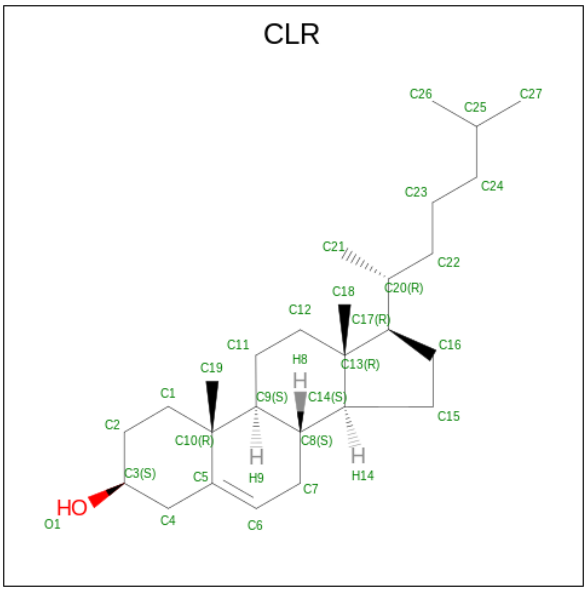
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| R | -93 | HIS | - | expression tag | UNP P0ABE7 |
| R | -86 | TRP | MET | conflict | UNP P0ABE7 |
| R | 9 | ILE | HIS | conflict | UNP P0ABE7 |
| R | 13 | LEU | - | linker | UNP P0ABE7 |
| R | 14 | ALA | - | linker | UNP P0ABE7 |
| R | 15 | SER | - | linker | UNP P0ABE7 |
| R | 16 | GLU | - | linker | UNP P0ABE7 |
| R | 17 | ASN | - | linker | UNP P0ABE7 |
| R | 18 | LEU | - | linker | UNP P0ABE7 |
| R | 19 | TYR | - | linker | UNP P0ABE7 |
| R | 20 | PHE | - | linker | UNP P0ABE7 |
| R | 21 | GLN | - | linker | UNP P0ABE7 |
| R | 24 | THR | ASN | conflict | UNP P08908 |
| R | 125 | TRP | LEU | conflict | UNP P08908 |

- Molecule 6 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).




| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 6 | R | 1 | Total | C | H | O | 0 |
| | | | 74 | 27 | 46 | 1 | |
| 6 | R | 1 | Total | C | H | O | 0 |
| | | | 74 | 27 | 46 | 1 | |
| 6 | R | 1 | Total | C | H | O | 0 |
| | | | 74 | 27 | 46 | 1 | |
| 6 | R | 1 | Total | C | H | O | 0 |
| | | | 74 | 27 | 46 | 1 | |

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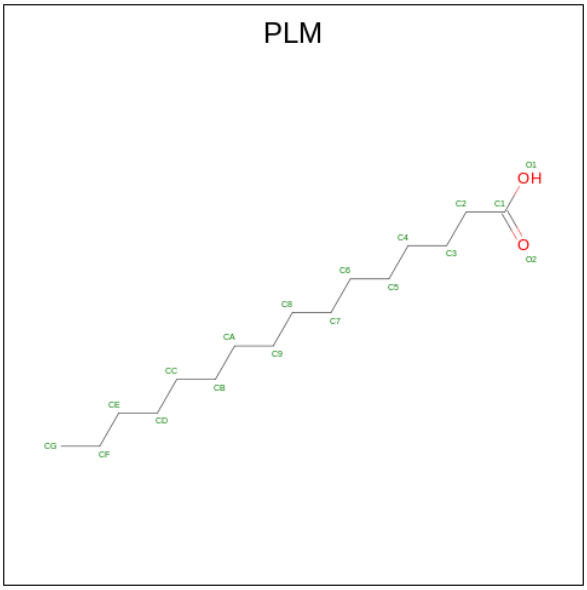
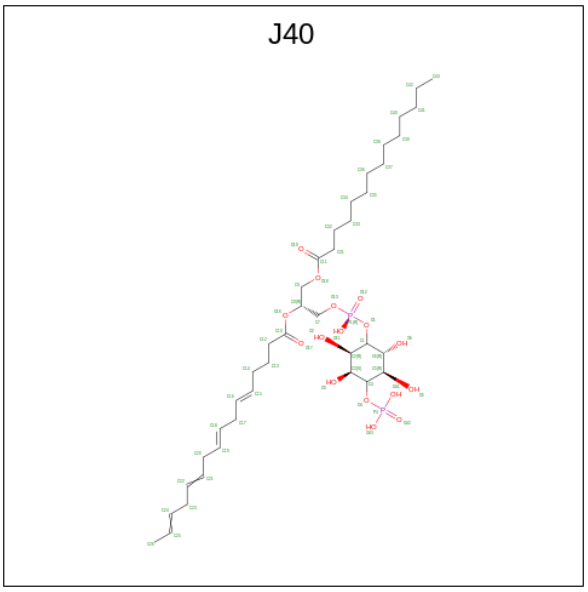
| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 6 | R | 1 | Total | C | H | O | 0 |
| | | | 74 | 27 | 46 | 1 | |

- Molecule 7 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



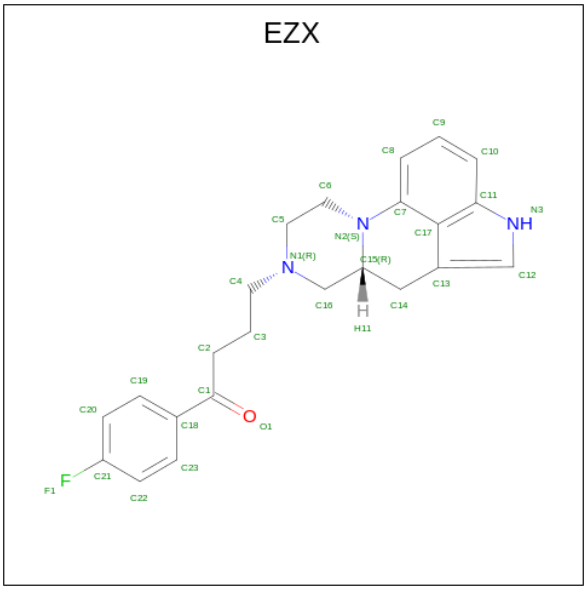

| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 7 | R | 1 | Total | C | H | O | 0 |
| | | | 49 | 16 | 31 | 2 | |
| 7 | R | 1 | Total | C | H | O | 0 |
| | | | 49 | 16 | 31 | 2 | |

- Molecule 8 is [(2R)-1-[oxidanyl-[(2R,3R,5S,6R)-2,3,5,6-tetrakis(oxidanyl)-4-phosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-3-tetradecanoyloxy-propan-2-yl] (5E,8E)-hexadeca-5,8,11,14-tetraenoate (three-letter code: J40) (formula: $C_{39}H_{68}O_{16}P_2$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 8 | R | 1 | Total | C | H | O | P | 0 |
| | | | 50 | 13 | 19 | 16 | 2 | |

- Molecule 9 is 1-(4-fluorophenyl)-4-[(7R)-2,5,11-triazatetracyclo[7.6.1.0^2,7.0^12,16]hexadeca-1(15),9,12(16),13-tetraen-5-yl]butan-1-one (three-letter code: EZX) (formula: $C_{23}H_{24}FN_3O$) (labeled as "Ligand of Interest" by depositor).



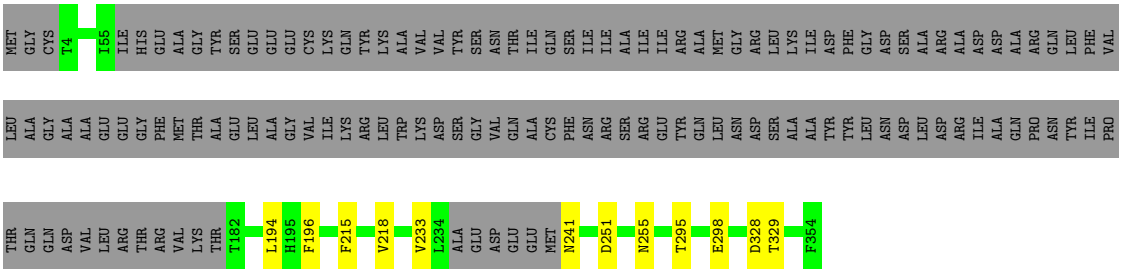

| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 9 | R | 1 | Total | C | F | H | N | O | 0 |
| | | | 52 | 23 | 1 | 24 | 3 | 1 | |

# 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.

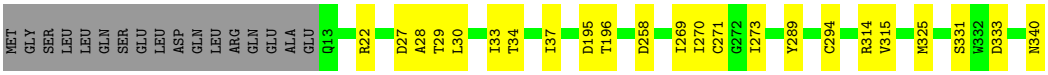
• Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1

Chain A:

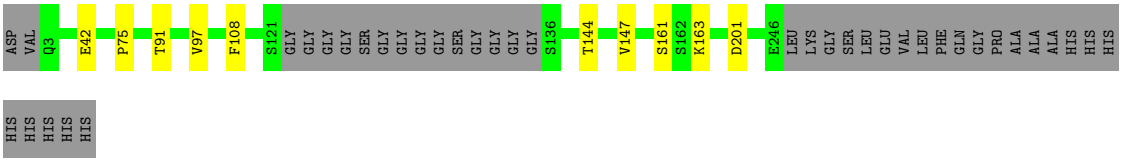

• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:

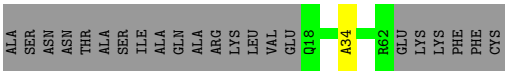

• Molecule 3: ScFv16

Chain E:

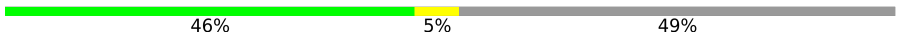

• Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

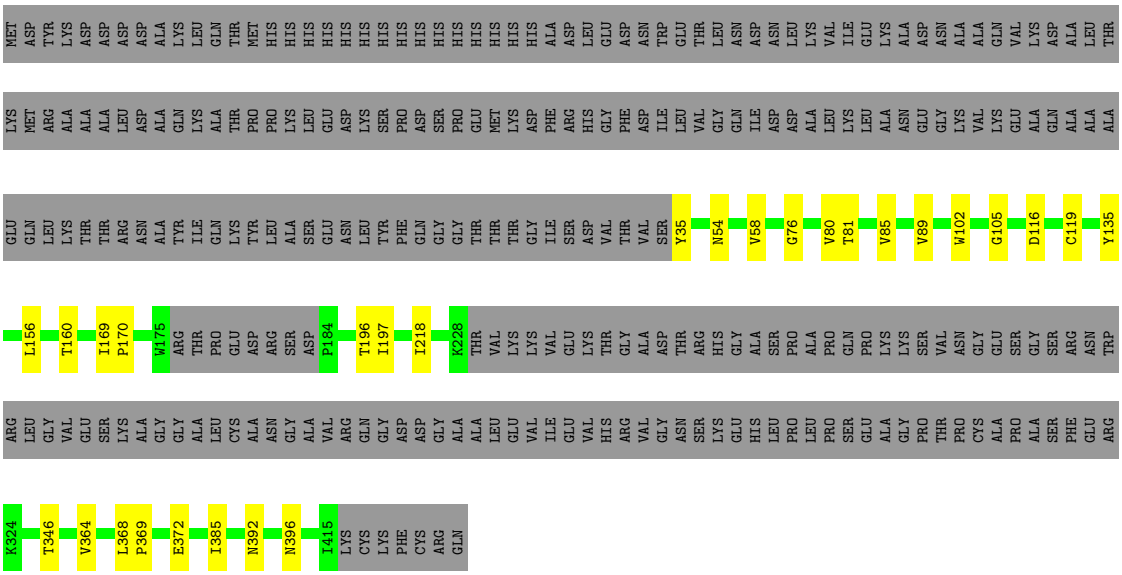
Chain G:


• Molecule 5: Soluble cytochrome b562,5-hydroxytryptamine receptor 1A

Chain R:




MET ASP TYR LYS ASP ASP ASP ASP ALA LYS LEU GLN THR MET HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS ALA ASP LEU GLU GLU ASP ASN TRP GLU THR LEU ASN ASP ASN LEU LYS VAL ILE GLU LYS ALA ASP ASN ALA ALA GLN VAL LYS ASP ALA LEU THR
LYS MET ARG ALA ALA ALA LEU ASP ALA GLN LYS ALA THR PRO PRO LYS LEU GLU ASP LYS SER PRO ASP SER PRO GLU MET LYS ASP PHE ARG HIS GLY PHE ASP ILE LEU VAL GLY GLN ILE ASP ASP ALA LEU LYS LEU ALA ASN GLU GLY LYS VAL LYS GLU ALA GLN ALA ALA ALA
GLU GLN LEU LYS THR THR ARG ASN ALA TYR ILE GLN LYS TYR LEU ALA SER GLU ASN LEU TYR PHE GLN GLY GLY THR THR THR GLY ILE SER ASP VAL THR VAL SER Y35 N54 V58 G76 V80 T81 V85 V89 W102 G105 D116 C119 Y135
L156 T160 I169 P170 W175 ARG THR PRO GLU ASP ARG SER ASP P184 T196 I197 I218 K228 THR VAL LYS LYS VAL GLU LYS THR GLY ALA ASP THR ARG HIS GLY ALA SER PRO ALA PRO GLN PRO LYS LYS SER VAL ASN GLY GLU SER GLY SER ARG ASN TRP
ARG LEU GLY VAL GLU SER LYS ALA GLY GLY ALA LEU CYS ALA ASN GLY ALA VAL ARG GLN GLY ASP ASP GLY ALA ALA LEU GLU VAL ILE GLU VAL HIS ARG VAL GLY ASN SER LYS GLU HIS LEU PRO LEU PRO PRO SER GLU ALA GLY PRO THR PRO CYS ALA PRO ALA SER PHE GLU ARG
K324 T346 V364 L368 P369 E372 I385 N392 N396 I415 LYS CYS LYS PHE CYS ARG GLN

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 175082 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | NONE | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 70 | Depositor |
| Minimum defocus (nm) | 1200 | Depositor |
| Maximum defocus (nm) | 2200 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLM, CLR, EZX, J40

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 | 0.24 | 0/1795 | 0.39 | 0/2407 |
| 2 | B | 0.23 | 0/2563 | 0.44 | 0/3475 |
| 3 | E | 0.26 | 0/1812 | 0.50 | 2/2456 (0.1%) |
| 4 | G | 0.24 | 0/353 | 0.40 | 0/477 |
| 5 | R | 0.25 | 0/2248 | 0.41 | 1/3058 (0.0%) |
| All | All | 0.25 | 0/8771 | 0.43 | 3/11873 (0.0%) |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | E | 75 | PRO | CA-N-CD | -9.30 | 98.48 | 111.50 |
| 5 | R | 369 | PRO | CA-N-CD | -5.34 | 104.03 | 111.50 |
| 3 | E | 75 | PRO | N-CD-CG | -5.17 | 95.44 | 103.20 |

There are no chirality outliers.

There are no planarity outliers.

## 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 | 1766 | 1771 | 1768 | 6 | 0 |
| 2 | B | 2516 | 2429 | 2427 | 16 | 0 |
| 3 | E | 1768 | 1703 | 1701 | 6 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 4 | G | 347 | 351 | 350 | 2 | 0 |
| 5 | R | 2197 | 2300 | 2298 | 15 | 0 |
| 6 | R | 140 | 230 | 230 | 40 | 0 |
| 7 | R | 36 | 62 | 62 | 0 | 0 |
| 8 | R | 31 | 19 | 0 | 1 | 0 |
| 9 | R | 28 | 24 | 0 | 0 | 0 |
| All | All | 8829 | 8889 | 8836 | 82 | 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 5.

The worst 5 of 82 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) |
|---|---|---|---|
| 6:R:504:CLR:C11 | 6:R:504:CLR:C12 | 1.74 | 1.64 |
| 6:R:506:CLR:C12 | 6:R:506:CLR:C11 | 1.74 | 1.63 |
| 6:R:503:CLR:C9 | 6:R:503:CLR:C11 | 1.75 | 1.62 |
| 6:R:501:CLR:C9 | 6:R:501:CLR:C11 | 1.75 | 1.61 |
| 6:R:503:CLR:C11 | 6:R:503:CLR:C12 | 1.74 | 1.61 |

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 PDB entries followed by that with respect to all EM entries.

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 | 213/354 (60%) | 212 (100%) | 1 (0%) | 0 | 100 | 100 |
| 2 | B | 326/345 (94%) | 318 (98%) | 8 (2%) | 0 | 100 | 100 |
| 3 | E | 226/269 (84%) | 223 (99%) | 3 (1%) | 0 | 100 | 100 |
| 4 | G | 43/67 (64%) | 43 (100%) | 0 | 0 | 100 | 100 |
| 5 | R | 272/544 (50%) | 271 (100%) | 1 (0%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| All | All | 1080/1579 (68%) | 1067 (99%) | 13 (1%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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 | 195/305 (64%) | 195 (100%) | 0 | 100 | 100 |
| 2 | B | 272/287 (95%) | 272 (100%) | 0 | 100 | 100 |
| 3 | E | 195/217 (90%) | 195 (100%) | 0 | 100 | 100 |
| 4 | G | 37/55 (67%) | 37 (100%) | 0 | 100 | 100 |
| 5 | R | 237/454 (52%) | 237 (100%) | 0 | 100 | 100 |
| All | All | 936/1318 (71%) | 936 (100%) | 0 | 100 | 100 |

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 340 | ASN |
| 5 | R | 126 | 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)

9 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 | $\#\|Z\| > 2$ |
| 6 | CLR | R | 502 | - | 31,31,31 | 4.14 | 15 (48%) | 48,48,48 | 1.51 | 8 (16%) |
| 9 | EZX | R | 509 | - | 30,32,32 | 4.75 | 17 (56%) | 35,46,46 | 2.26 | 13 (37%) |
| 8 | J40 | R | 508 | - | 31,31,57 | 1.24 | 3 (9%) | 43,46,72 | 1.53 | 8 (18%) |
| 6 | CLR | R | 501 | - | 31,31,31 | 4.19 | 15 (48%) | 48,48,48 | 1.53 | 8 (16%) |
| 6 | CLR | R | 503 | - | 31,31,31 | 4.15 | 15 (48%) | 48,48,48 | 1.49 | 10 (20%) |
| 6 | CLR | R | 506 | - | 31,31,31 | 4.16 | 15 (48%) | 48,48,48 | 1.47 | 6 (12%) |
| 6 | CLR | R | 504 | - | 31,31,31 | 4.15 | 15 (48%) | 48,48,48 | 1.54 | 10 (20%) |
| 7 | PLM | R | 505 | - | 17,17,17 | 0.92 | 1 (5%) | 17,17,17 | 0.74 | 2 (11%) |
| 7 | PLM | R | 507 | - | 17,17,17 | 0.93 | 1 (5%) | 17,17,17 | 0.74 | 1 (5%) |

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 |
|---|---|---|---|---|---|---|---|
| 6 | CLR | R | 502 | - | - | 1/10/68/68 | 0/4/4/4 |
| 9 | EZX | R | 509 | - | - | 6/10/31/31 | 0/4/5/5 |
| 8 | J40 | R | 508 | - | - | 12/25/49/77 | 0/1/1/1 |
| 6 | CLR | R | 501 | - | - | 4/10/68/68 | 0/4/4/4 |
| 6 | CLR | R | 503 | - | - | 0/10/68/68 | 0/4/4/4 |
| 6 | CLR | R | 506 | - | - | 1/10/68/68 | 0/4/4/4 |
| 6 | CLR | R | 504 | - | - | 0/10/68/68 | 0/4/4/4 |
| 7 | PLM | R | 505 | - | - | 2/15/15/15 | - |

*Continued on next page...*

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 7 | PLM | R | 507 | - | - | 2/15/15/15 | - |

The worst 5 of 97 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 9 | R | 509 | EZX | C7-C17 | -18.93 | 1.12 | 1.43 |
| 6 | R | 502 | CLR | C11-C9 | 13.20 | 1.75 | 1.53 |
| 6 | R | 504 | CLR | C11-C9 | 13.19 | 1.75 | 1.53 |
| 6 | R | 501 | CLR | C11-C9 | 13.18 | 1.75 | 1.53 |
| 6 | R | 506 | CLR | C11-C9 | 13.18 | 1.75 | 1.53 |

The worst 5 of 66 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | R | 504 | CLR | C15-C14-C8 | -5.54 | 109.96 | 119.08 |
| 9 | R | 509 | EZX | C6-N2-C7 | -5.52 | 108.33 | 118.64 |
| 9 | R | 509 | EZX | C8-C7-N2 | -5.39 | 119.31 | 123.40 |
| 6 | R | 506 | CLR | C15-C14-C8 | -5.23 | 110.47 | 119.08 |
| 6 | R | 503 | CLR | C15-C14-C8 | -5.14 | 110.62 | 119.08 |

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 8 | R | 508 | J40 | C7-O13-P1-O12 |
| 8 | R | 508 | J40 | C7-O13-P1-O11 |
| 8 | R | 508 | J40 | C7-O13-P1-O1 |
| 8 | R | 508 | J40 | C8-C7-O13-P1 |
| 8 | R | 508 | J40 | C2-C1-O1-P1 |

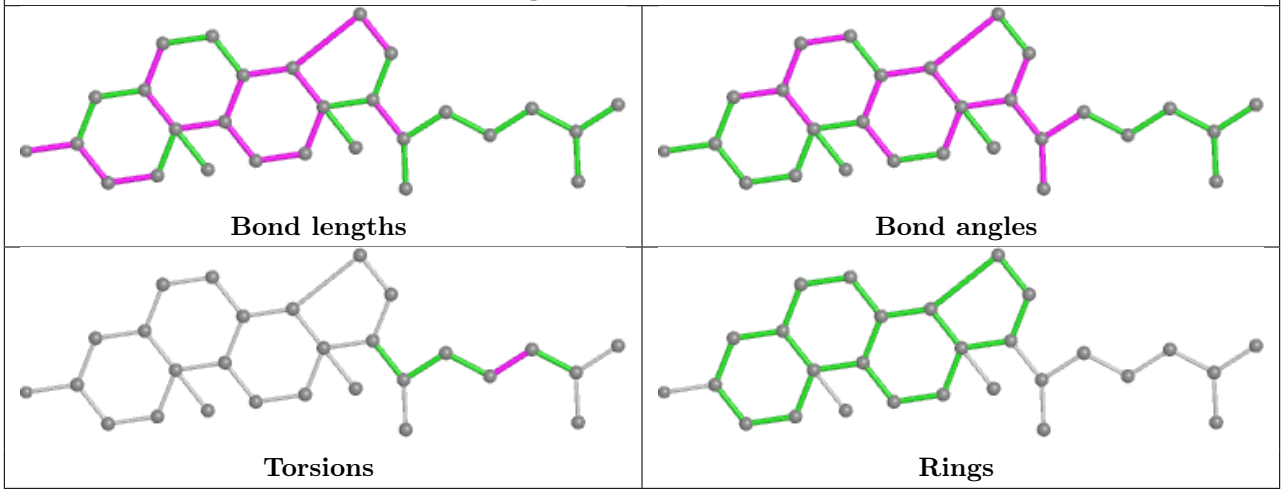
There are no ring outliers.

6 monomers are involved in 41 short contacts:

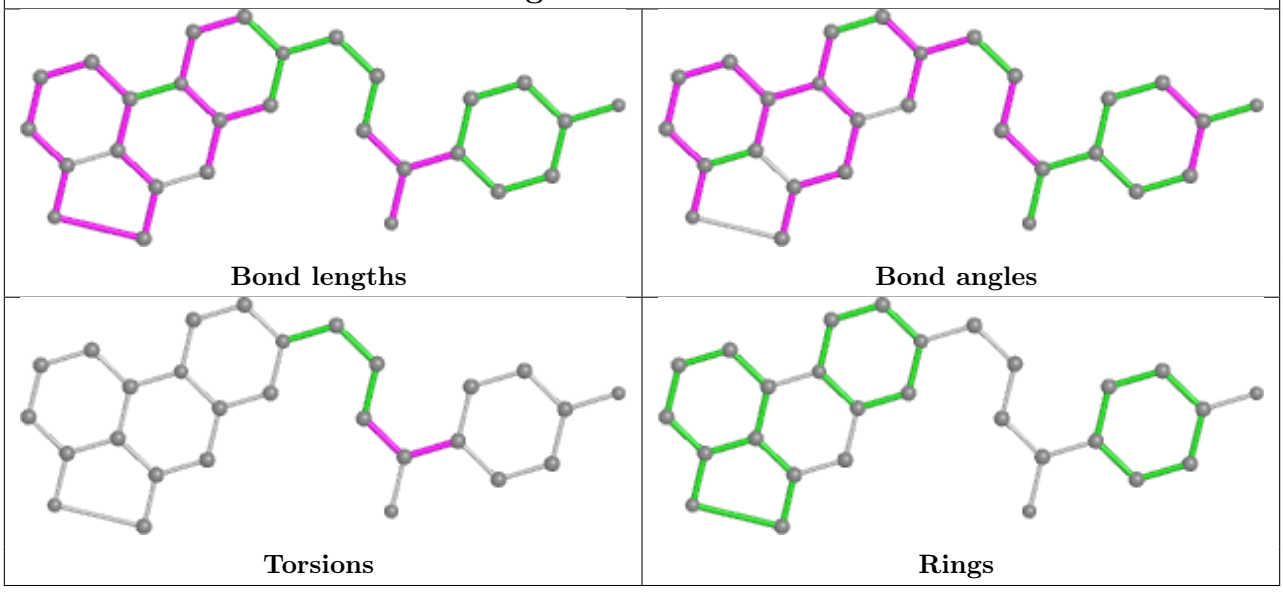
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 6 | R | 502 | CLR | 9 | 0 |
| 8 | R | 508 | J40 | 1 | 0 |
| 6 | R | 501 | CLR | 7 | 0 |
| 6 | R | 503 | CLR | 8 | 0 |
| 6 | R | 506 | CLR | 8 | 0 |
| 6 | R | 504 | CLR | 8 | 0 |

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 then 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.

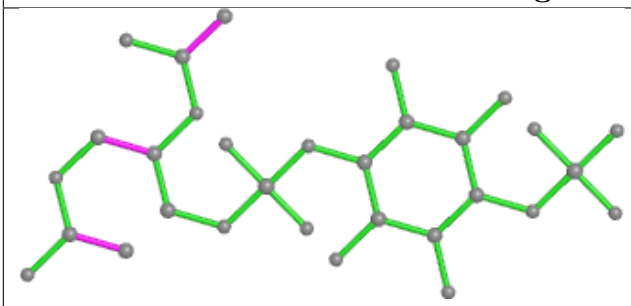
**Ligand CLR R 502**



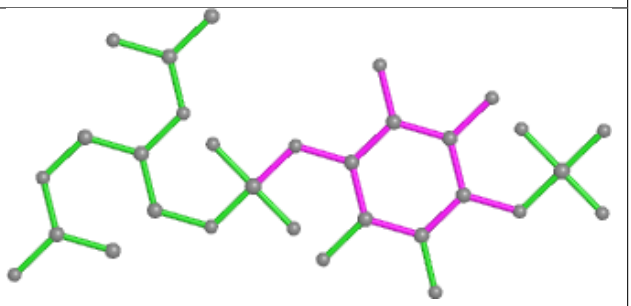

**Ligand EZX R 509**



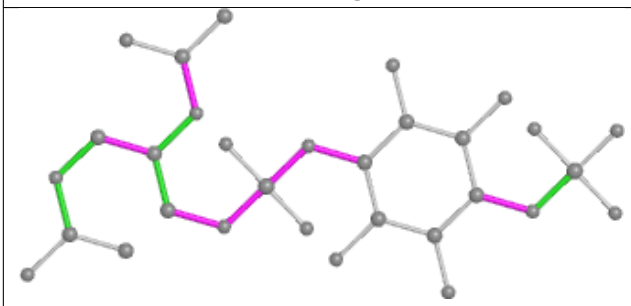
## Ligand J40 R 508



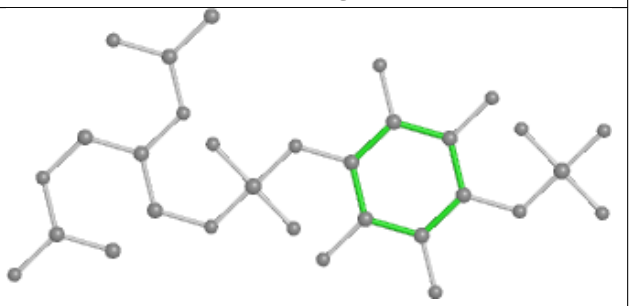
Bond lengths



Bond angles

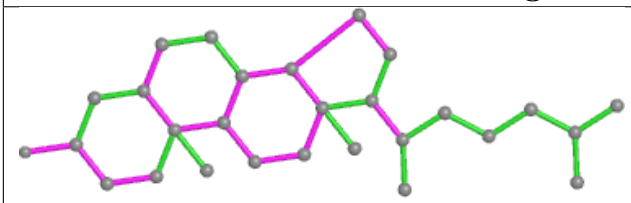


Torsions

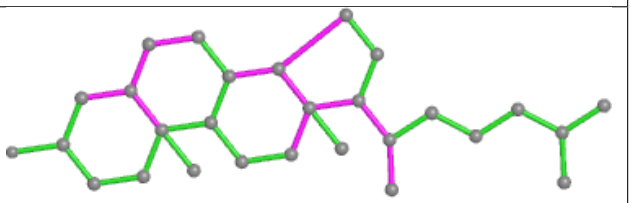


Rings

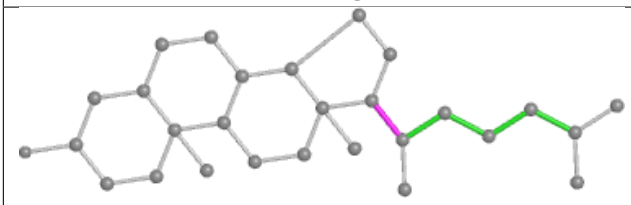
## Ligand CLR R 501



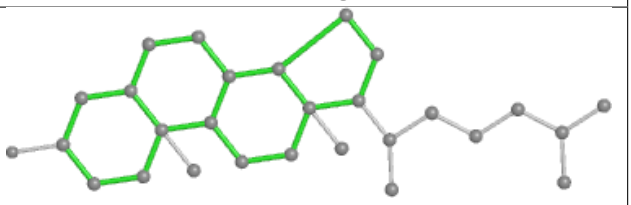
Bond lengths



Bond angles

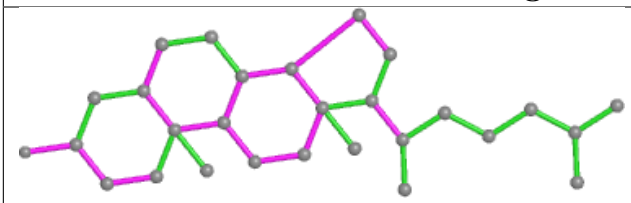


Torsions

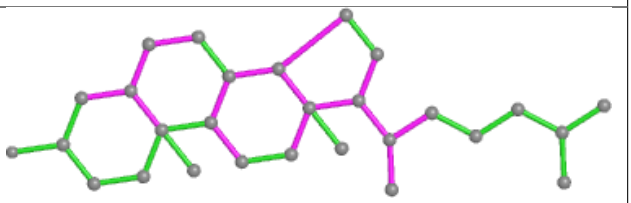


Rings

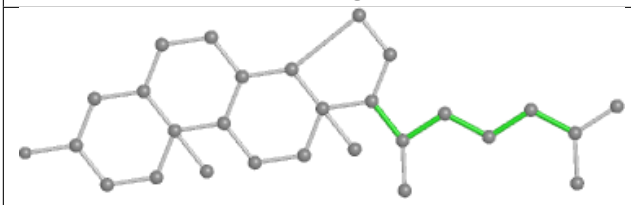
## Ligand CLR R 503



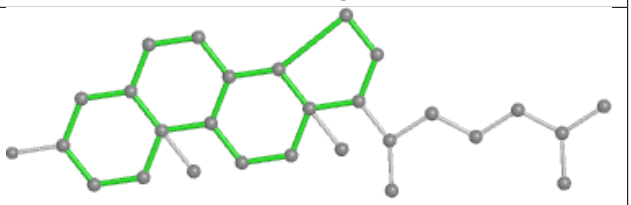
Bond lengths



Bond angles

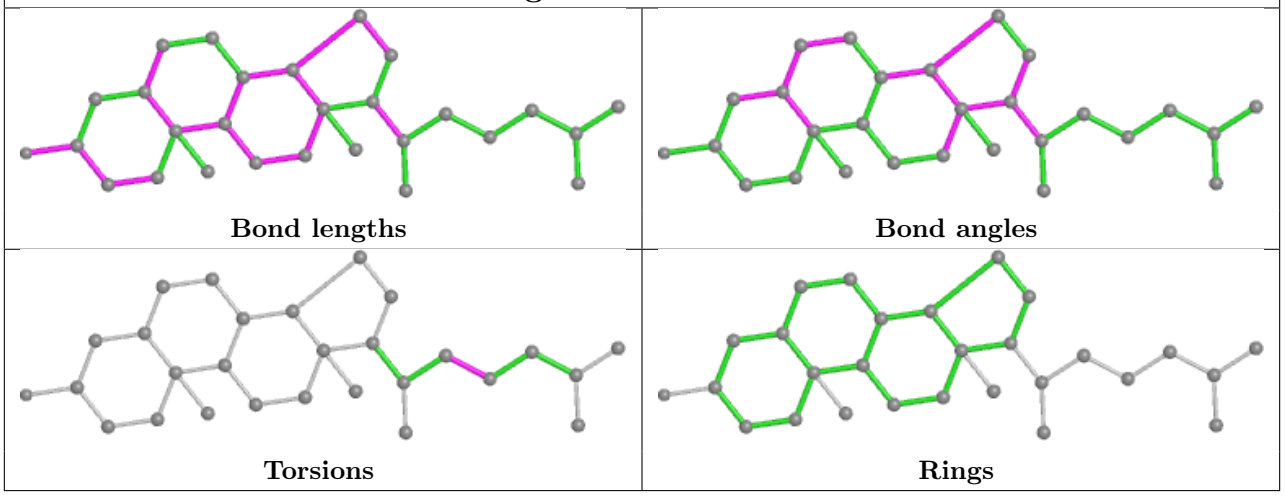


Torsions

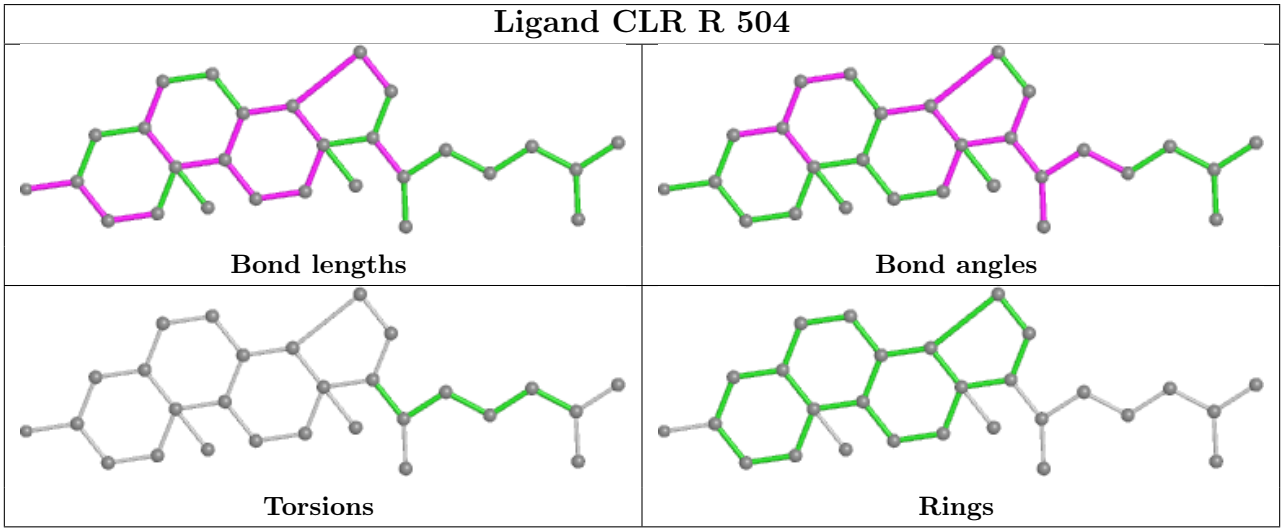


Rings

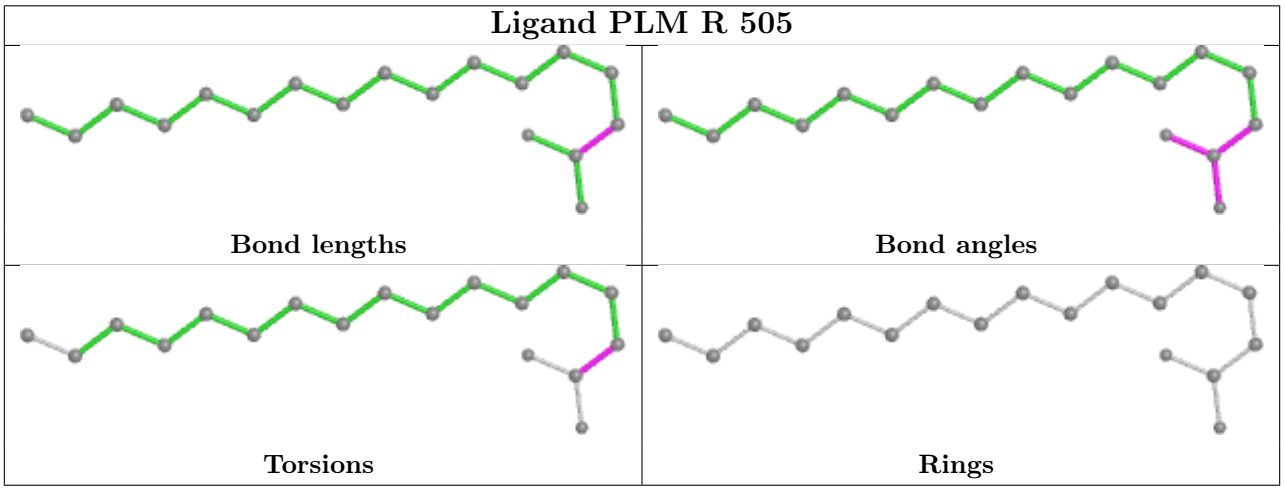
## Ligand CLR R 506



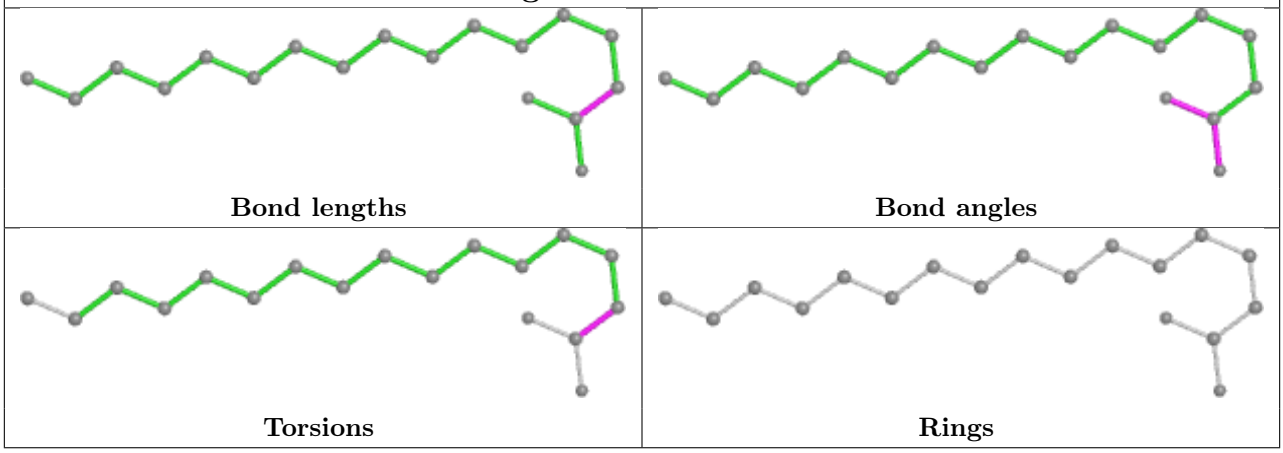

## Ligand CLR R 504




## Ligand PLM R 505



**Ligand PLM R 507**




## 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.