



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 14, 2023 – 04:13 PM EDT

PDB ID : 1RDT
Title : Crystal Structure of a new rexinoid bound to the RXRalpha ligand binding domain in the RXRalpha/PPARgamma heterodimer
Authors : Haffner, C.D.; Lenhard, J.M.; Miller, A.B.; McDougald, D.L.; Dwornik, K.; Ittoop, O.R.; Gampe Jr., R.T.; Xu, H.E.; Blanchard, S.; Montana, V.G.
Deposited on : 2003-11-06
Resolution : 2.40 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 : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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) : 2.35

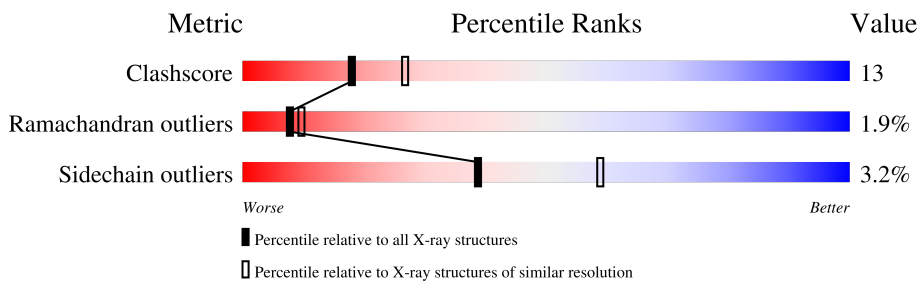
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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	242	
2	B	25	
3	D	284	
4	E	23	

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
5	L79	A	463	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4027 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 Retinoic acid receptor RXR-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	211	1644	1054	285	295	10	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	221	MET	-	cloning artifact	UNP P19793
A	222	LYS	-	cloning artifact	UNP P19793
A	223	LYS	-	cloning artifact	UNP P19793
A	224	GLY	-	cloning artifact	UNP P19793

- Molecule 2 is a protein called LxxLL motif coactivator.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	9	77	50	17	10	0	0	0

- Molecule 3 is a protein called Peroxisome proliferator activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	253	1998	1288	327	376	7	0	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	194	MET	-	cloning artifact	UNP P37231
D	195	LYS	-	cloning artifact	UNP P37231
D	196	LYS	-	cloning artifact	UNP P37231
D	197	GLY	-	cloning artifact	UNP P37231
D	198	HIS	-	cloning artifact	UNP P37231
D	199	HIS	-	cloning artifact	UNP P37231

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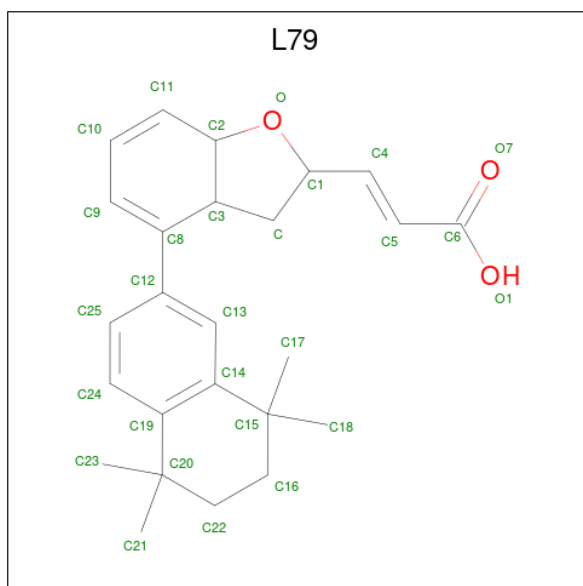
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Chain	Residue	Modelled	Actual	Comment	Reference
D	200	HIS	-	cloning artifact	UNP P37231
D	201	HIS	-	cloning artifact	UNP P37231
D	202	HIS	-	cloning artifact	UNP P37231
D	203	HIS	-	cloning artifact	UNP P37231
D	204	GLY	-	cloning artifact	UNP P37231
D	205	ARG	-	cloning artifact	UNP P37231
D	206	ALA	-	cloning artifact	UNP P37231

- Molecule 4 is a protein called LxxLL motif coactivator.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	E	7	34	20	7	7	0	0	0

- Molecule 5 is (S)-(2E)-3[4-(5,5,8,8-TETRAMETHYL-5,6,7,8-TETRAHYDRO-2-NAPHTHALENYL)TETRAHYDRO-1-BENZOFURAN-2-YL]-2-PROPENOIC ACID (three-letter code: L79) (formula: C₂₅H₃₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	28	25	3	0	0

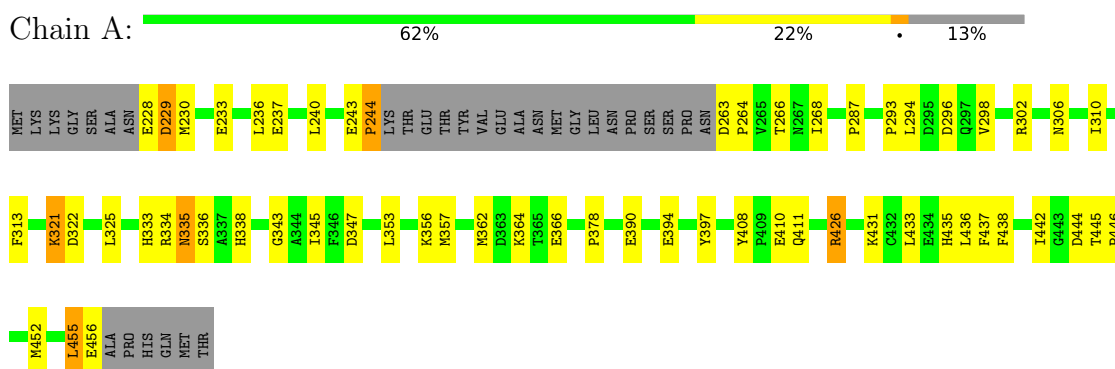
- Molecule 6 is 2-(2-BENZOYL-PHENYLAMINO)-3-{4-[2-(5-METHYL-2-PHENYL-OXAZOL-4-YL)-ETHOXY]-PHENYL}-PROPIONIC ACID (three-letter code: 570) (formula: C₃₄H₃₀N₂O₅).

3 Residue-property plots [i](#)

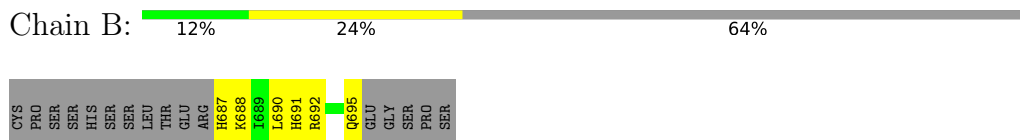
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

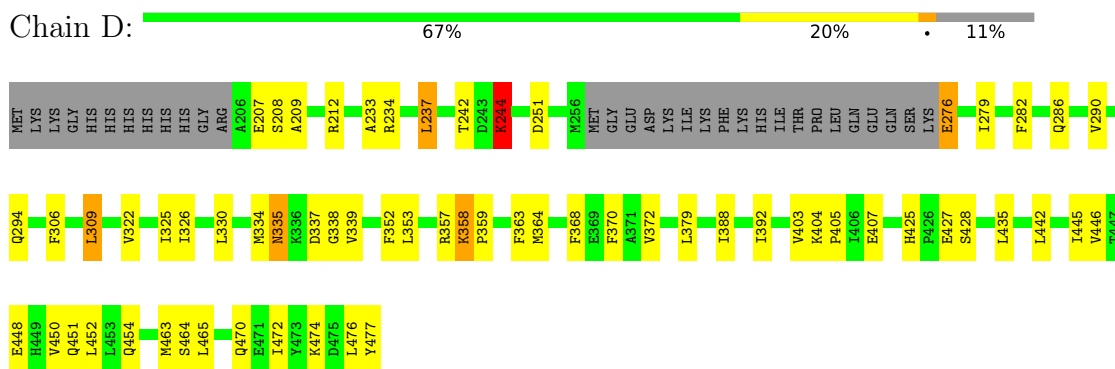
- Molecule 1: Retinoic acid receptor RXR-alpha



- Molecule 2: LxxLL motif coactivator



- Molecule 3: Peroxisome proliferator activated receptor gamma



- Molecule 4: LxxLL motif coactivator



ASN	LEU	VAL	PRO	ASP	ALA	ALA	SER	LYS	HIS	K67	L73	ARG	GLY	GLY	SER	GLY	SER
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.69Å 54.58Å 211.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	97.1 (20.00-2.40)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNX 2000	Depositor
R, R_{free}	0.221 , 0.259	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4027	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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: L79, 570

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	0.26	0/1676	0.52	0/2261
2	B	0.27	0/78	0.54	0/104
3	D	0.26	0/2031	0.50	0/2739
4	E	0.43	0/33	0.33	0/44
All	All	0.27	0/3818	0.51	0/5148

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	1644	0	1662	48	2
2	B	77	0	80	7	2
3	D	1998	0	2028	53	0
4	E	34	0	12	0	0
5	A	28	0	26	2	0
6	D	41	0	29	0	0
7	A	72	0	0	2	0
7	B	2	0	0	0	0
7	D	123	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	8	0	0	0	0
All	All	4027	0	3837	103	2

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 13.

The worst 5 of 103 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)
3:D:358:LYS:HB3	3:D:359:PRO:HD2	1.30	1.06
3:D:242:THR:HG22	7:D:566:HOH:O	1.55	1.04
3:D:358:LYS:HB3	3:D:359:PRO:CD	1.90	1.02
1:A:233:GLU:HG3	7:A:103:HOH:O	0.84	1.00
3:D:357:ARG:NH2	3:D:358:LYS:HD2	2.00	0.76

All (2) 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:240:LEU:CD1	2:B:692:ARG:NE[3_645]	1.66	0.54
1:A:240:LEU:CD1	2:B:692:ARG:CD[3_645]	1.76	0.44

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	207/242 (86%)	189 (91%)	13 (6%)	5 (2%)	6 6
2	B	7/25 (28%)	7 (100%)	0	0	100 100
3	D	249/284 (88%)	236 (95%)	9 (4%)	4 (2%)	9 13
4	E	5/23 (22%)	5 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	468/574 (82%)	437 (93%)	22 (5%)	9 (2%)	8 10

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	321	LYS
1	A	446	PRO
3	D	358	LYS
1	A	444	ASP
3	D	244	LYS

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 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	175/208 (84%)	167 (95%)	8 (5%)	27 43
2	B	8/24 (33%)	8 (100%)	0	100 100
3	D	219/254 (86%)	214 (98%)	5 (2%)	50 70
All	All	402/486 (83%)	389 (97%)	13 (3%)	39 59

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	455	LEU
3	D	237	LEU
3	D	335	ASN
3	D	276	GLU
3	D	309	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	294	GLN
3	D	308	ASN

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Mol	Chain	Res	Type
3	D	451	GLN
3	D	335	ASN
1	A	335	ASN

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](#)

2 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
5	L79	A	463	-	31,31,31	4.01	17 (54%)	40,48,48	3.03	11 (27%)
6	570	D	478	-	40,45,45	1.83	13 (32%)	47,61,61	1.26	5 (10%)

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
5	L79	A	463	-	3/3/7/12	4/9/50/50	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	570	D	478	-	-	3/25/30/30	0/5/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	463	L79	C3-C2	-11.14	1.39	1.54
5	A	463	L79	C9-C8	9.77	1.53	1.35
5	A	463	L79	C10-C11	8.52	1.53	1.33
5	A	463	L79	C-C3	-7.32	1.39	1.54
5	A	463	L79	C-C1	-6.00	1.39	1.54

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	463	L79	O-C2-C11	11.44	126.85	110.47
5	A	463	L79	O-C1-C4	8.21	127.84	109.29
5	A	463	L79	O-C2-C3	6.27	108.77	100.65
5	A	463	L79	C16-C15-C14	4.55	117.50	110.16
5	A	463	L79	C22-C20-C19	4.33	117.14	110.16

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	463	L79	C3
5	A	463	L79	C2
5	A	463	L79	C1

5 of 7 torsion outliers are listed below:

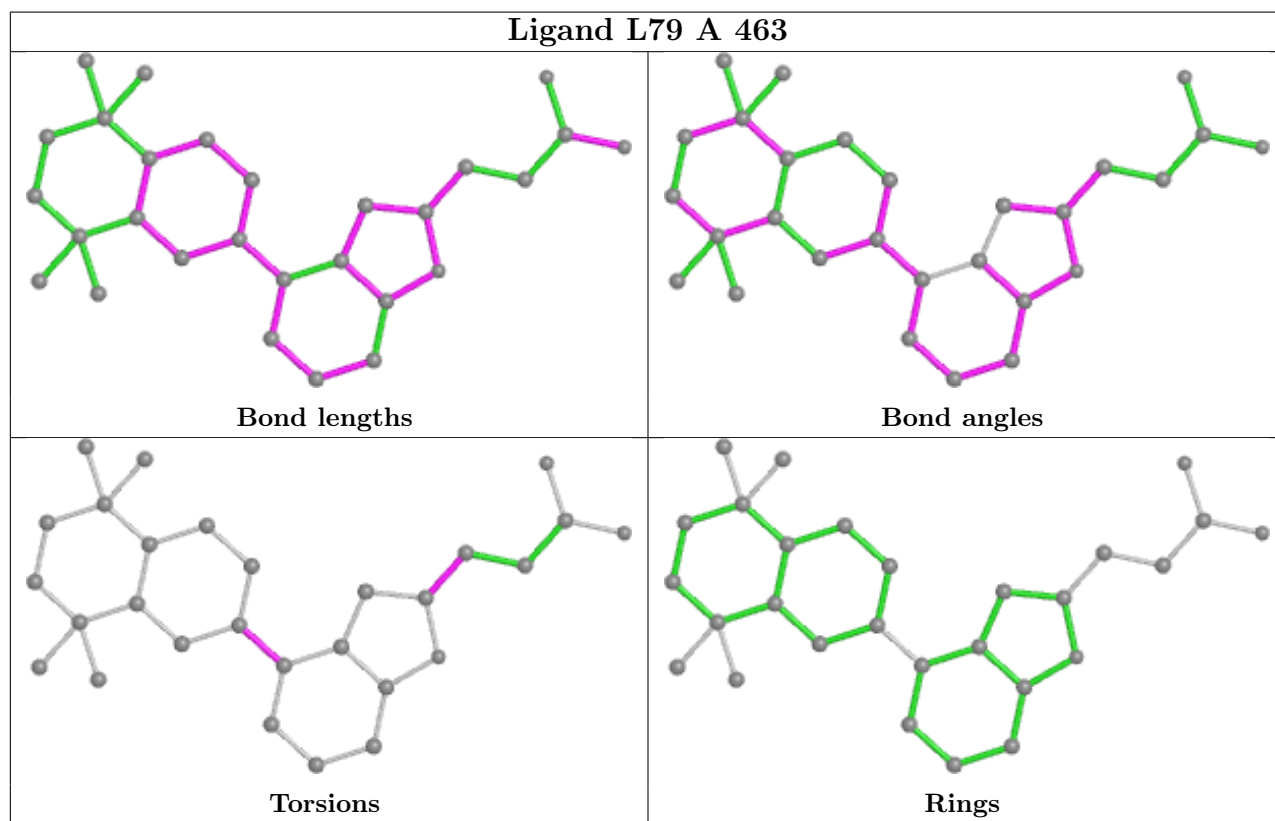
Mol	Chain	Res	Type	Atoms
5	A	463	L79	O-C1-C4-C5
6	D	478	570	OH-C3A-C3B-C3C
6	D	478	570	CE1-CZ-OH-C3A
6	D	478	570	CE2-CZ-OH-C3A
5	A	463	L79	C13-C12-C8-C9

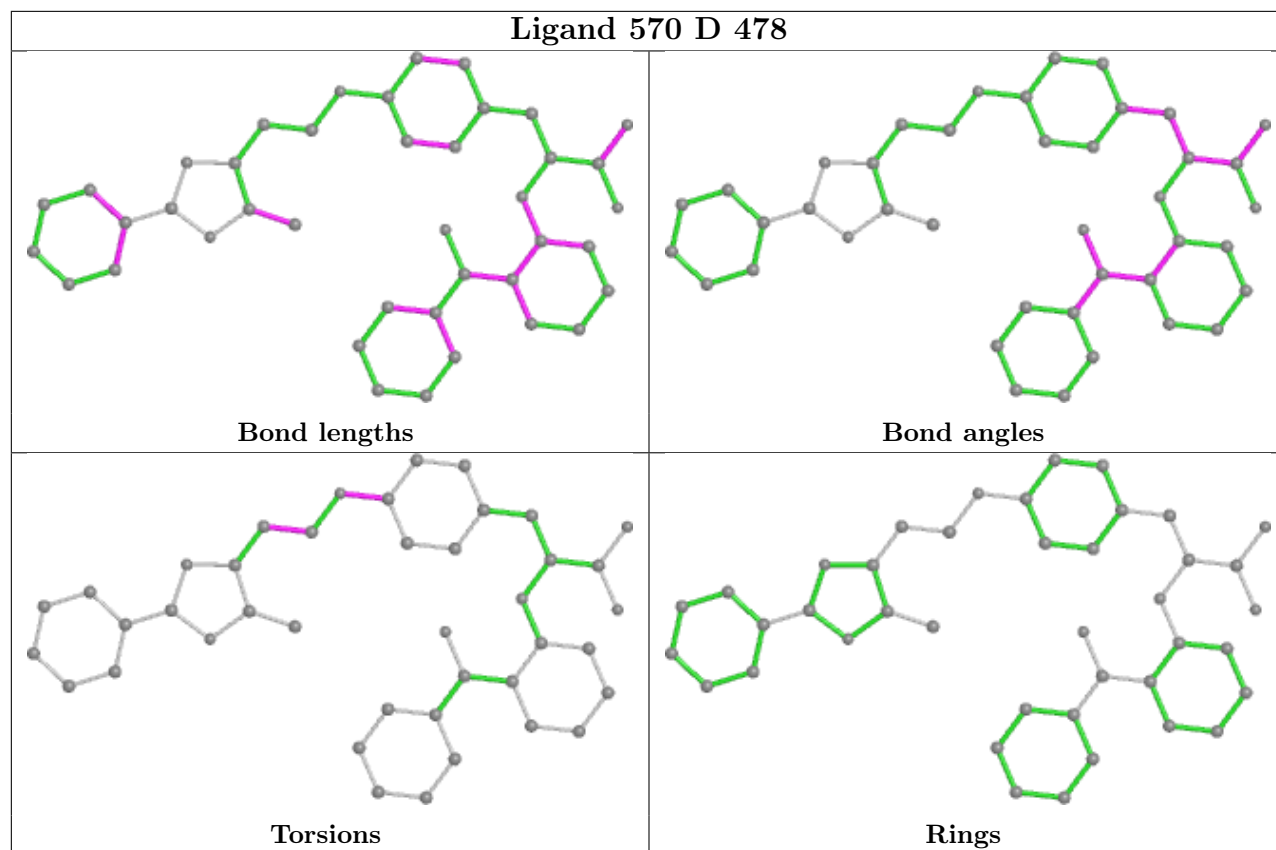
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	463	L79	2	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.