WORLDWIDE wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 18, 2023 – 12:29 PM EDT

PDB ID	:	1UHL
Title	:	Crystal structure of the LXRalfa-RXRbeta LBD heterodimer
Authors	:	Svensson, S.; Ostberg, T.; Jacobsson, M.; Norstrom, C.; Stefansson, K.; Hallen, D.; Johansson, I.C.; Zachrisson, K.; Ogg, D.; Jendeberg, L.
Deposited on	:	2003-07-03
Resolution	:	2.90 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

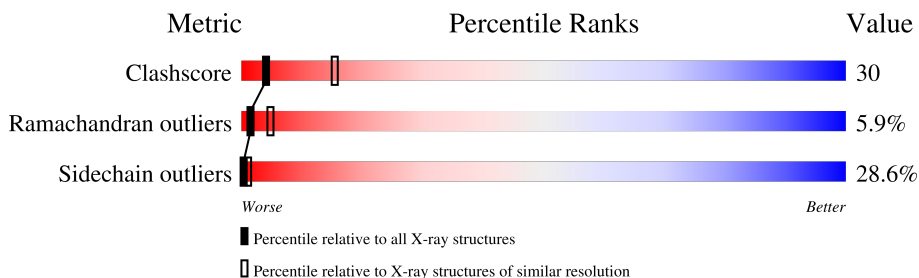|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.90 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	Percentile Ranks	Value
Clashscore		30
Ramachandran outliers		5.9%
Sidechain outliers		28.6%

Worse   *Better*

▮ Percentile relative to all X-ray structures
🄳 Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	236	38% 37% 14% • 9%
2	B	242	33% 38% 16% • 10%
3	C	10	30% 30% 10% 20% 10%
3	D	10	30% 50% 10% 10%

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
4	MEI	A	1001	-	-	X	-

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 3707 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-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1698	1085	294	309	10			

- Molecule 2 is a protein called Oxysterols receptor LXR-alpha.

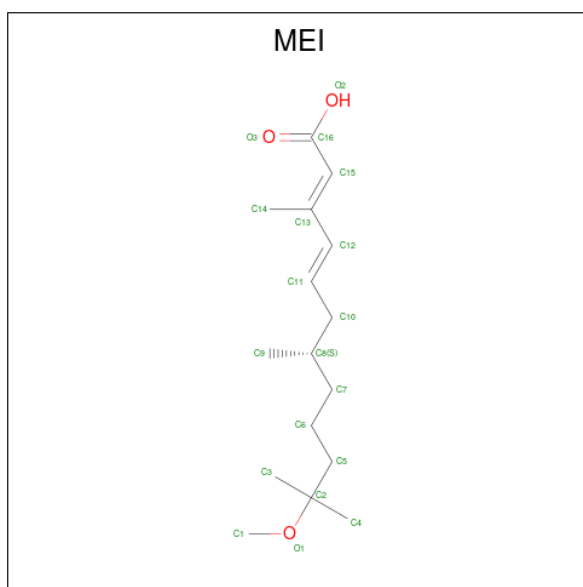| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	219	Total	C	N	O	S	0	0	0
			1777	1132	311	326	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	206	MET	-	expression tag	UNP Q13133

- Molecule 3 is a protein called 10-mer peptide from Nuclear receptor coactivator 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			81	53	18	10			
3	D	10	Total	C	N	O	0	0	0
			89	57	19	13			

- Molecule 4 is (2E,4E)-11-METHOXY-3,7,11-TRIMETHYLDODECA-2,4-DIENOIC ACID (three-letter code: MEI) (formula: $C_{16}H_{28}O_3$).

MEI

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 19	C 16	O 3	0	0

- Molecule 5 is N-(2,2,2-TRIFLUOROETHYL)-N-{4-[2,2,2-TRIFLUORO-1-HYDROXY-1-(TRIFLUOROMETHYL)ETHYL]PHENYL}BENZENESULFONAMIDE (three-letter code: 444) (formula: $C_{17}H_{12}F_9NO_3S$).

444
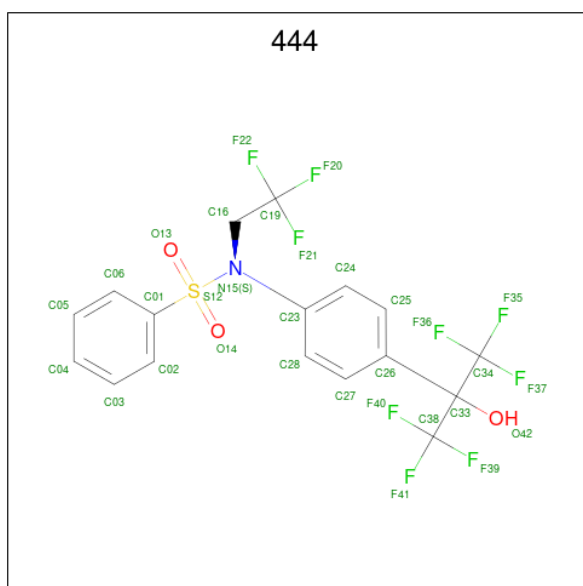
| Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total 31	C 17	F 9	N 1	O 3	S 1	0	0

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	11	Total 11	O 11	0	0
6	B	1	Total 1	O 1	0	0

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: Retinoic acid receptor RXR-beta
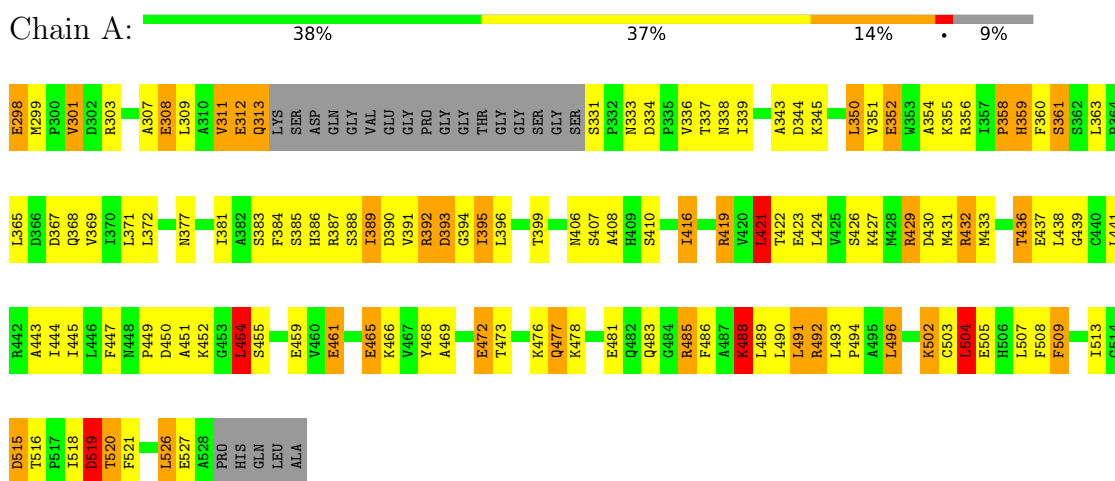
Chain A:

• Molecule 2: Oxysterols receptor LXR-alpha
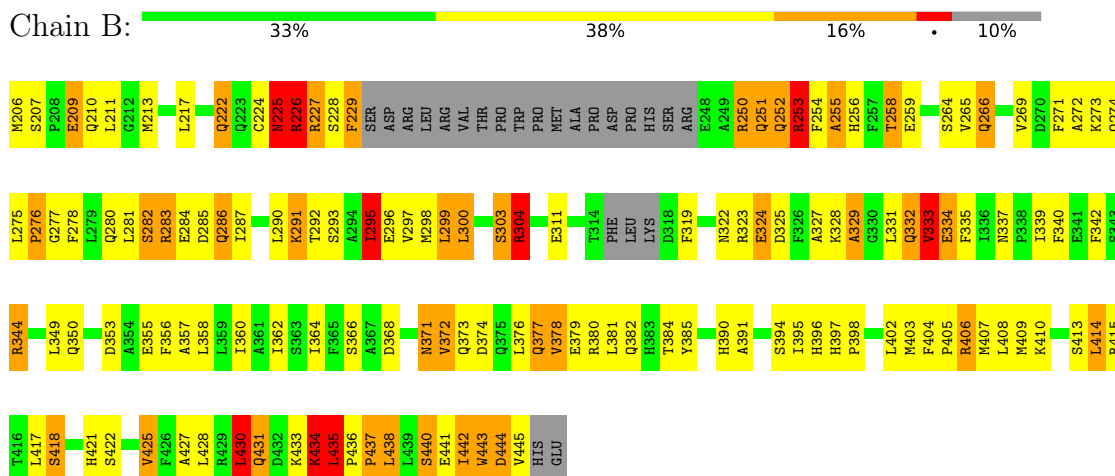
Chain B:

• Molecule 3: 10-mer peptide from Nuclear receptor coactivator 2

Chain C:

H604 K605 I606 L607 H608 R609 L610 L611 Q612 ASP
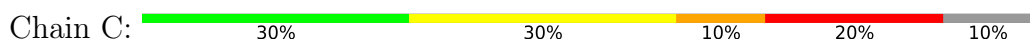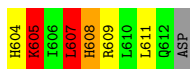
• Molecule 3: 10-mer peptide from Nuclear receptor coactivator 2

Chain D:

30%   50%   10%   10%

H604 K605 I606 L607 H608 L611 Q612 D613

4 Data and refinement statistics ⓘ

Xtriage (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	67.63Å 89.00Å 90.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.65 – 2.90	Depositor
% Data completeness (in resolution range)	99.9 (19.65-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.219 , 0.326	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3707	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 444, MEI

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	1.30	6/1729 (0.3%)	1.45	21/2336 (0.9%)
2	B	1.27	6/1810 (0.3%)	1.39	13/2443 (0.5%)
3	C	1.26	0/82	1.39	1/108 (0.9%)
3	D	1.18	0/90	1.21	1/119 (0.8%)
All	All	1.28	12/3711 (0.3%)	1.41	36/5006 (0.7%)

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
2	B	0	5

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	465	GLU	CD-OE1	6.13	1.32	1.25
2	B	340	PHE	CE2-CZ	5.96	1.48	1.37
1	A	426	SER	CB-OG	5.94	1.50	1.42
2	B	443	TRP	CB-CG	5.94	1.60	1.50
1	A	416	ILE	CA-CB	5.87	1.68	1.54

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	429	ARG	NE-CZ-NH1	11.38	125.99	120.30
2	B	444	ASP	CB-CG-OD2	10.14	127.43	118.30
1	A	387	ARG	NE-CZ-NH1	-9.49	115.56	120.30
2	B	253	ARG	NE-CZ-NH1	8.76	124.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	491	LEU	CA-CB-CG	-8.23	96.36	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	226	ARG	Peptide
2	B	334	GLU	Peptide
2	B	431	GLN	Peptide
2	B	434	LYS	Peptide
2	B	435	LEU	Peptide

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	1698	0	1734	88	0
2	B	1777	0	1776	132	0
3	C	81	0	91	4	0
3	D	89	0	95	8	0
4	A	19	0	27	11	0
5	B	31	0	12	3	0
6	A	11	0	0	0	0
6	B	1	0	0	0	0
All	All	3707	0	3735	223	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 30.

The worst 5 of 223 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)
2:B:295:ILE:CD1	2:B:295:ILE:H	1.54	1.20
1:A:419:ARG:HG2	1:A:419:ARG:HH11	1.05	1.13
2:B:295:ILE:H	2:B:295:ILE:HD12	1.22	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:406:ARG:HG3	2:B:406:ARG:HH11	1.29	0.97
2:B:349:LEU:HD21	2:B:406:ARG:HD2	1.47	0.95

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 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	210/236 (89%)	181 (86%)	21 (10%)	8 (4%)	3	13
2	B	213/242 (88%)	166 (78%)	31 (15%)	16 (8%)	1	2
3	C	7/10 (70%)	4 (57%)	2 (29%)	1 (14%)	0	0
3	D	8/10 (80%)	5 (62%)	2 (25%)	1 (12%)	0	0
All	All	438/498 (88%)	356 (81%)	56 (13%)	26 (6%)	1	5

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	SER
1	A	520	THR
2	B	225	ASN
2	B	252	GLN
2	B	311	GLU

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	187/201 (93%)	134 (72%)	53 (28%)	0	1
2	B	196/219 (90%)	142 (72%)	54 (28%)	0	1
3	C	9/10 (90%)	5 (56%)	4 (44%)	0	0
3	D	10/10 (100%)	6 (60%)	4 (40%)	0	0
All	All	402/440 (91%)	287 (71%)	115 (29%)	0	1

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	226	ARG
3	C	609	ARG
2	B	287	ILE
3	C	608	HIS
2	B	428	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	377	GLN
2	B	382	GLN
3	D	608	HIS
2	B	397	HIS
3	D	604	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\#|Z| > 2$
4	MEI	A	1001	-	18,18,18	0.69	0	21,23,23	3.94	7 (33%)
5	444	B	1002	-	31,32,32	2.48	5 (16%)	52,52,52	3.24	16 (30%)

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
4	MEI	A	1001	-	-	10/20/20/20	-
5	444	B	1002	-	-	7/45/45/45	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1002	444	C01-S12	-10.09	1.62	1.76
5	B	1002	444	C16-C19	5.77	1.58	1.50
5	B	1002	444	O13-S12	4.36	1.48	1.43
5	B	1002	444	C34-C33	-2.37	1.50	1.54
5	B	1002	444	C27-C26	2.03	1.42	1.39

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(º)	Ideal(º)
4	A	1001	MEI	C11-C12-C13	-13.42	105.61	125.89
5	B	1002	444	O14-S12-O13	-10.10	103.16	119.52
5	B	1002	444	O14-S12-N15	8.20	116.41	106.71
5	B	1002	444	C16-N15-S12	7.47	127.41	117.00
5	B	1002	444	C19-C16-N15	7.10	119.04	112.14

There are no chirality outliers.
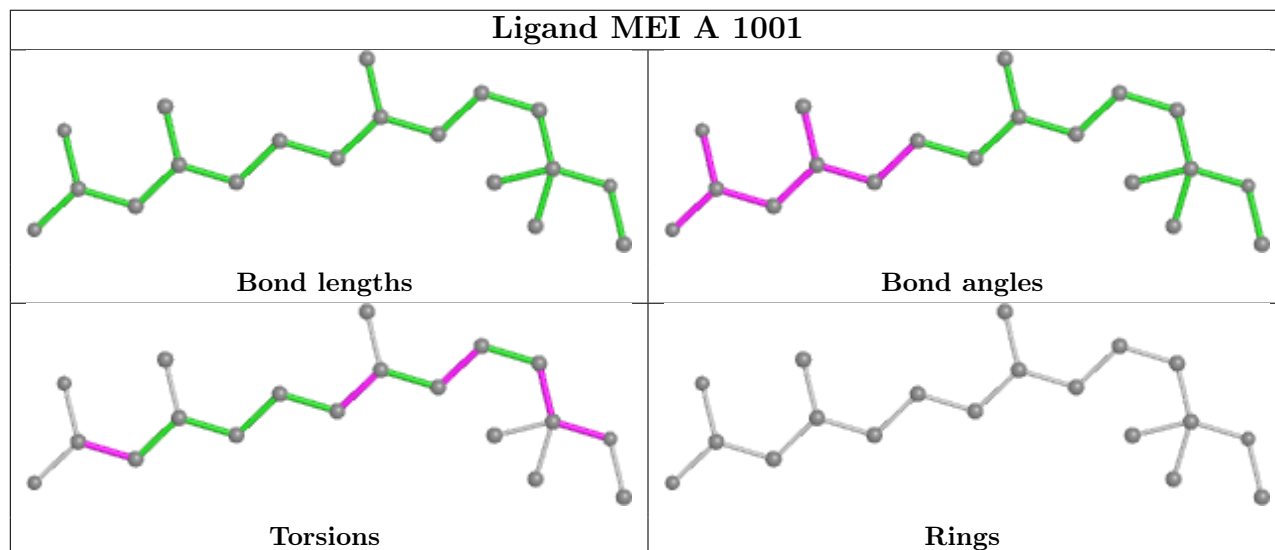
5 of 17 torsion outliers are listed below:

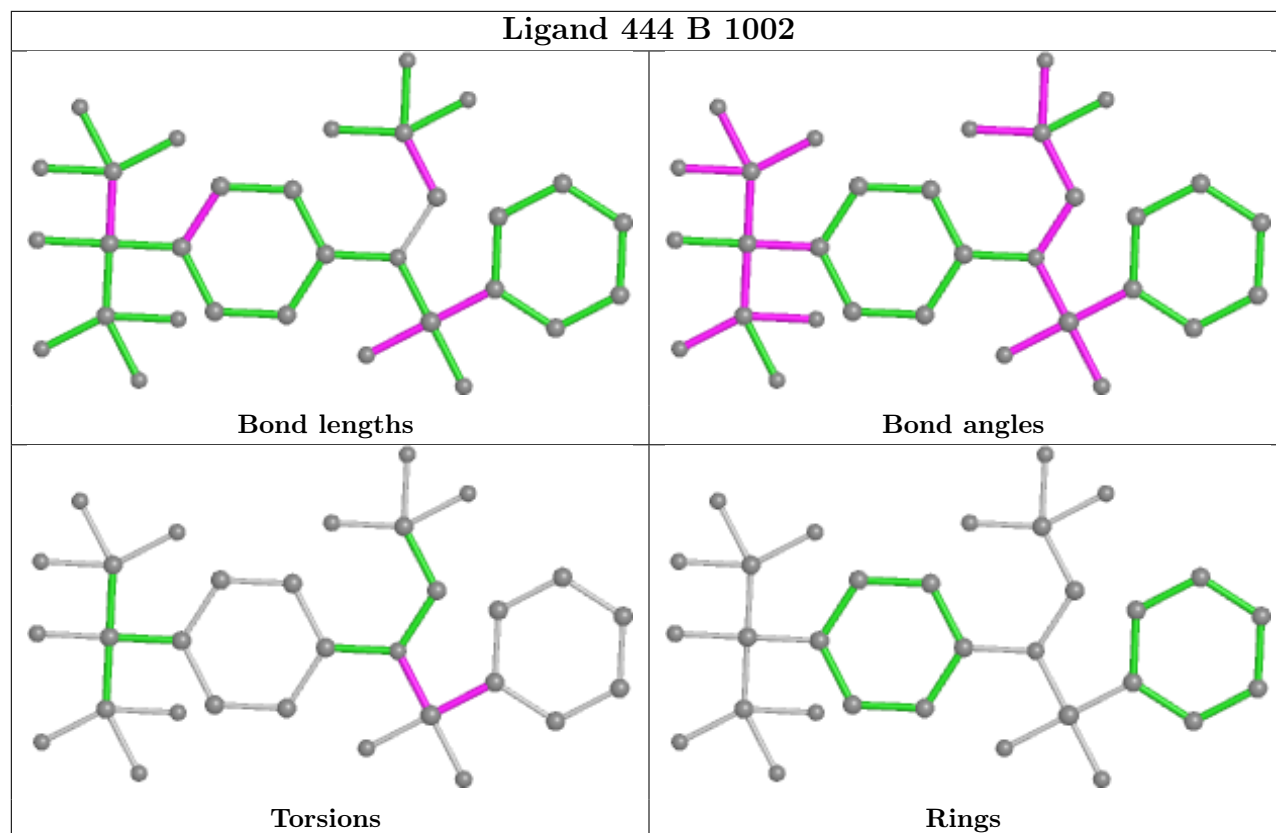| Mol	Chain	Res	Type	Atoms
4	A	1001	MEI	C3-C2-C5-C6
4	A	1001	MEI	C4-C2-C5-C6
4	A	1001	MEI	C11-C10-C8-C9
4	A	1001	MEI	C13-C15-C16-O2
4	A	1001	MEI	C13-C15-C16-O3

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	MEI	11	0
5	B	1002	444	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 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 MEI A 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand 444 B 1002

Bond lengths

Bond angles

Torsions

Rings

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.