

wwPDB X-ray Structure Validation Summary Report (i)

Sep 16, 2021 – 02:15 pm BST

PDB ID : 7ORC

Title : Human Aldehyde Oxidase in complex with Raloxifene Authors : Mota, C.; Coelho, C.; Santos Silva, T.; Romao, M.J.

Deposited on : 2021-06-05

Resolution : 2.70 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 (i) symbol.

The following versions of software and data (see references (1)) 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)

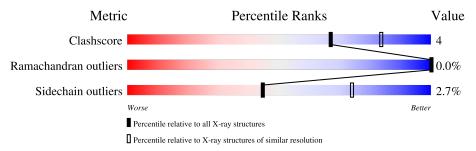
Validation Pipeline (wwPDB-VP) : 2.23.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 2.70 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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	1338	86%	11%	• • •
1	В	1338	84%	12%	• • •



2 Entry composition (i)

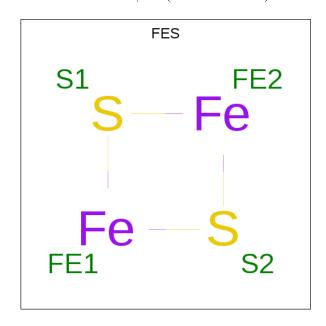
There are 8 unique types of molecules in this entry. The entry contains 20656 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aldehyde oxidase.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
1	A	1295	Total 10056	C 6389	N 1732	O 1855	S 80	0	0	0
1	В	1299	Total 10083	C 6407	N 1737	O 1859	S 80	0	0	0

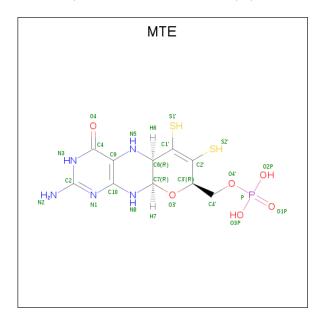
• Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe S 4 2 2	0	0
2	A	1	Total Fe S 4 2 2	0	0
2	В	1	Total Fe S 4 2 2	0	0
2	В	1	Total Fe S 4 2 2	0	0

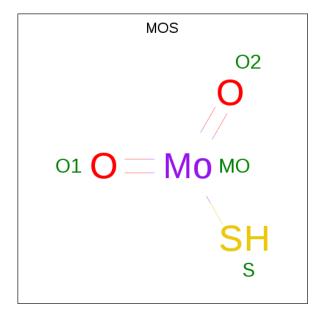


• Molecule 3 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (three-letter code: MTE) (formula: $C_{10}H_{14}N_5O_6PS_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf		
2	3 A	Λ	1	Total	С	N	О	Р	S	0	0
, J		1	24	10	5	6	1	2	0		
9	3 B	D	1	Total	С	N	О	Р	S	0	0
3		1	24	10	5	6	1	2	0	U	

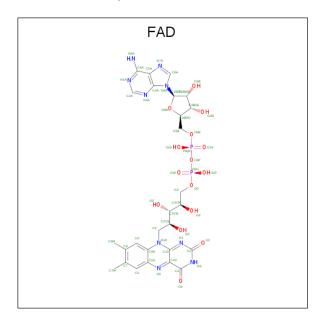
• Molecule 4 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula: $HMoO_2S$).





Mol	Chain	Residues	${f Atoms}$				ZeroOcc	AltConf	
1	Δ	1	Total	Мо	Ο	S	n	0	
	T 1	1	4	1	2	1	U		
4	D	1	Total	Мо	Ο	S	0	0	
4	4 B	1	4	1	2	1	U	0	

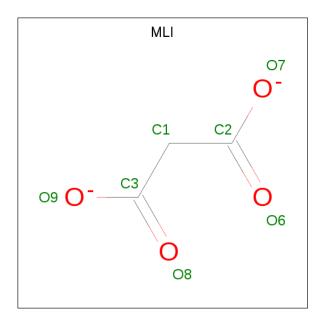
 \bullet Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2).$



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf			
5	Λ.	Λ 1		С	N	О	Р	0	0		
'	9 A	1	53	27	9	15	2	U			
5	5 B	D	D	1	Total	С	N	О	Р	0	0
		1	53	27	9	15	2	U	0		

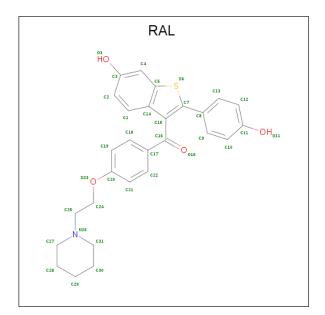
• Molecule 6 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 3 4	0	0
6	A	1	Total C O 7 3 4	0	0
6	A	1	Total C O 7 3 4	0	0
6	В	1	Total C O 7 3 4	0	0

• Molecule 7 is RALOXIFENE (three-letter code: RAL) (formula: $C_{28}H_{27}NO_4S$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	
7	Λ	1	Total	С	Ν	О	S	0	0	
'	A	1	34	28	1	4	1	U		
7	Λ	1	Total	С	N	О	S	0	0	
'	Α	1	34	28	1	4	1	U		
7	D	1	Total	С	N	О	S	0	0	
'	Б	1	34	28	1	4	1	U		
7	D	1	Total	С	N	О	S	0	0	
'	7 B	1	34	28	1	4	1	0		

• Molecule 8 is water.

Mol	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
8	A	80	Total O 80 80	0	0
8	В	95	Total O 95 95	0	0

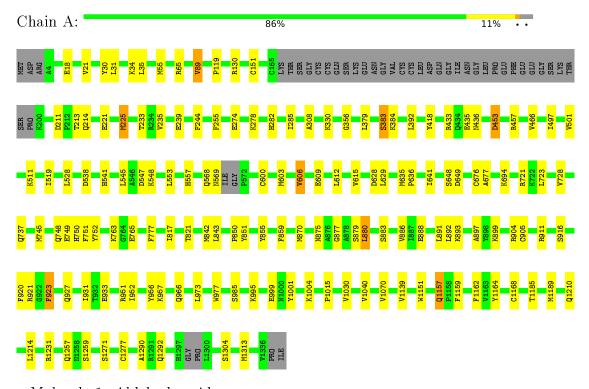


3 Residue-property plots (i)

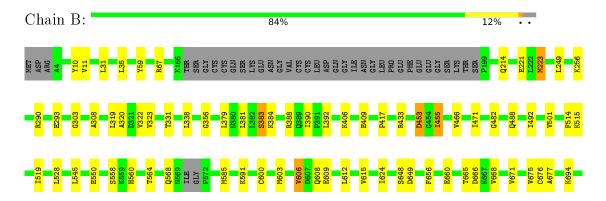
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

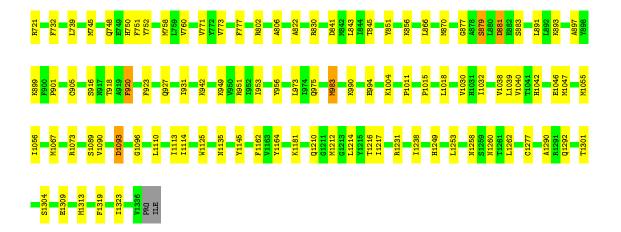
• Molecule 1: Aldehyde oxidase



• Molecule 1: Aldehyde oxidase









4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 43 21 2	Depositor	
Cell constants	149.03Å 149.03Å 268.73Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	48.85 - 2.70	Depositor	
% Data completeness	99.9 (48.85-2.70)	Depositor	
(in resolution range)	,	Беровног	
R_{merge}	(Not available)	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	PHENIX 1.19_4092	Depositor	
R, R_{free}	0.219 , 0.252	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	20656	wwPDB-VP	
Average B, all atoms (Å ²)	52.0	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: RAL, FES, MLI, MOS, MTE, FAD

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		
MIOI		RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.25	0/10269	0.48	0/13886	
1	В	0.25	0/10299	0.47	0/13928	
All	All	0.25	0/20568	0.47	0/27814	

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)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	10056	0	10099	76	0
1	В	10083	0	10131	87	0
2	A	8	0	0	1	0
2	В	8	0	0	0	0
3	A	24	0	10	0	0
3	В	24	0	10	0	0
4	A	4	0	0	0	0
4	В	4	0	0	0	0
5	A	53	0	31	0	0
5	В	53	0	31	0	0
6	A	21	0	6	0	0

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-	110116	picolous	puyc

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	В	7	0	2	0	0
7	A	68	0	52	1	0
7	В	68	0	52	1	0
8	A	80	0	0	0	0
8	В	95	0	0	1	0
All	All	20656	0	20424	161	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 4.

The worst 5 of 161 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{array}{c} ext{Clash} \ ext{overlap } (ext{Å}) \end{array}$
1:B:615:VAL:HB	1:B:676:CYS:HB2	1.75	0.68
1:A:89:VAL:HG21	1:A:119:PRO:HB3	1.74	0.67
1:B:1018:LEU:HD21	1:B:1090:VAL:HG21	1.77	0.67
1:A:433:ARG:HH12	1:A:436:ASN:HB3	1.61	0.65
1:A:211:ASP:OD2	1:A:214:GLN:HG2	1.97	0.64

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	${f Analysed}$	Favoured	Allowed	Outliers	Perce	\mathbf{ntiles}
1	A	$1287/1338 \; (96\%)$	1244 (97%)	42 (3%)	1 (0%)	51	78
1	В	1293/1338~(97%)	1249 (97%)	44 (3%)	0	100	100
All	All	2580/2676~(96%)	2493 (97%)	86 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	453	ASP

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	Rotameric Outliers	
1	A	1100/1136~(97%)	1074 (98%)	26 (2%)	49 77
1	В	1103/1136 (97%)	1069 (97%)	34 (3%)	40 69
All	All	$2203/2272 \ (97\%)$	2143 (97%)	60 (3%)	44 74

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	223	MET
1	В	1231	ARG
1	В	560	HIS
1	В	1093	ASP
1	В	1301	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	GLN
1	A	1210	GLN
1	A	1335	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)

18 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).

Mal	Т	Chain	Dag	T ! 1-	Вс	ond leng	$_{ m ths}$	В	ond ang	;les
Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	$\mid \# Z > 2$
6	MLI	A	1408	_	0,6,6	0.00	-	0,7,7	0.00	-
7	RAL	A	1410	_	33,38,38	0.55	1 (3%)	43,53,53	0.94	2 (4%)
3	MTE	В	1403	4	21,26,26	0.97	1 (4%)	21,40,40	2.00	7 (33%)
5	FAD	В	1405	-	51,58,58	1.08	2 (3%)	60,89,89	1.74	7 (11%)
3	MTE	A	1403	4	21,26,26	0.99	1 (4%)	21,40,40	2.02	8 (38%)
5	FAD	A	1405	-	51,58,58	1.08	2 (3%)	60,89,89	1.73	7 (11%)
4	MOS	В	1404	3	0,3,3	0.00	-	-		
6	MLI	A	1407	-	0,6,6	0.00	-	0,7,7	0.00	-
2	FES	A	1402	1	0,4,4	0.00	-	_		
6	MLI	В	1406	_	0,6,6	0.00	-	0,7,7	0.00	_
2	FES	В	1401	1	0,4,4	0.00	-	_		
2	FES	A	1401	1	0,4,4	0.00	_	_		
4	MOS	A	1404	3	0,3,3	0.00	_	_		
7	RAL	A	1409	-	33,38,38	0.56	1 (3%)	43,53,53	0.85	2 (4%)
7	RAL	В	1407	_	33,38,38	0.57	1 (3%)	43,53,53	0.83	2 (4%)
7	RAL	В	1408	-	33,38,38	0.53	1 (3%)	43,53,53	0.89	2 (4%)
2	FES	В	1402	1	0,4,4	0.00	-	-		
6	MLI	A	1406	-	0,6,6	0.00	-	0,7,7	0.00	_

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	MLI	Α	1408	-	-	0/0/4/4	-
7	RAL	A	1410	_	-	5/15/26/26	0/5/5/5
3	MTE	В	1403	4	-	1/6/34/34	0/3/3/3
5	FAD	В	1405	-	-	1/30/50/50	0/6/6/6
3	MTE	A	1403	4	-	1/6/34/34	0/3/3/3
5	FAD	A	1405	-	-	1/30/50/50	0/6/6/6
6	MLI	A	1407	-	-	0/0/4/4	-
6	MLI	В	1406	-	-	0/0/4/4	-
2	FES	A	1402	1	-	-	0/1/1/1
7	RAL	A	1409	_	-	3/15/26/26	0/5/5/5
2	FES	A	1401	1	-	-	0/1/1/1
2	FES	В	1401	1	-	-	0/1/1/1
7	RAL	В	1407	_	-	4/15/26/26	0/5/5/5
7	RAL	В	1408	_	-	4/15/26/26	0/5/5/5
2	FES	В	1402	1	-	-	0/1/1/1
6	MLI	A	1406	_	_	0/0/4/4	_

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	${f Atoms}$	\mathbf{Z}	${f Observed(\AA)}$	$\operatorname{Ideal}(ext{ ilde{A}})$
5	В	1405	FAD	C4X-C10	5.71	1.44	1.38
5	A	1405	FAD	C4X-C10	5.67	1.44	1.38
3	A	1403	MTE	C4-N3	3.35	1.38	1.33
3	В	1403	MTE	C4-N3	3.33	1.38	1.33
5	A	1405	FAD	C4-N3	2.71	1.37	1.33

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

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
5	В	1405	FAD	C4-N3-C2	8.13	122.00	115.14
5	A	1405	FAD	C4-N3-C2	8.03	121.92	115.14
5	В	1405	FAD	C10-C4X-N5	5.26	124.90	121.26
3	A	1403	MTE	C4-C9-C10	5.25	119.23	114.57
5	A	1405	FAD	C10-C4X-N5	5.24	124.89	121.26

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1403	MTE	C3'-C4'-O4'-P
3	В	1403	MTE	C3'-C4'-O4'-P
7	В	1407	RAL	O23-C24-C25-N26

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Mol	Chain	${f Res}$	Type	Atoms
7	В	1408	RAL	C21-C20-O23-C24
7	В	1407	RAL	C19-C20-O23-C24

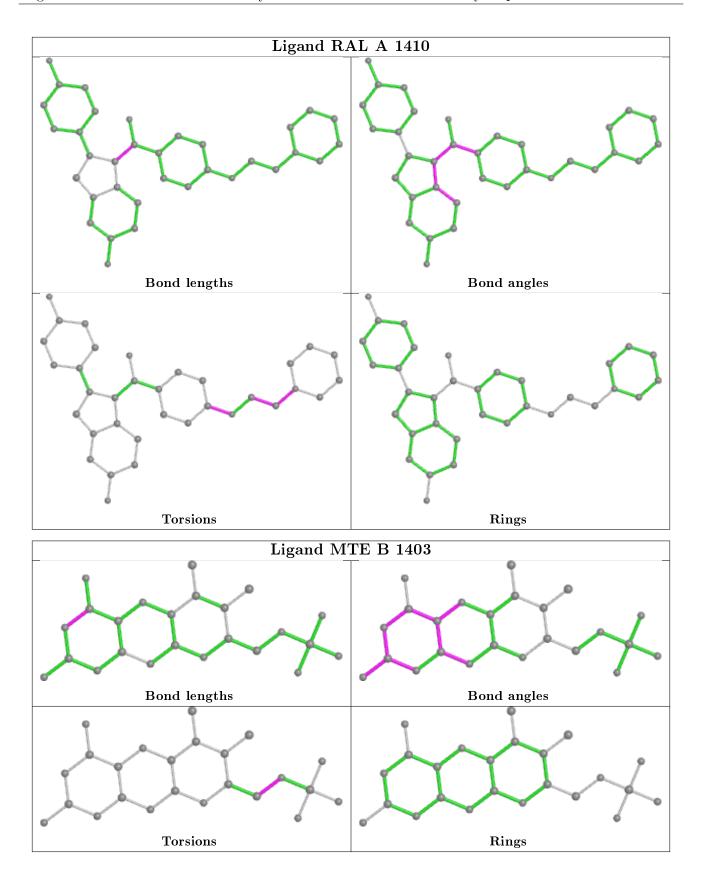
There are no ring outliers.

3 monomers are involved in 3 short contacts:

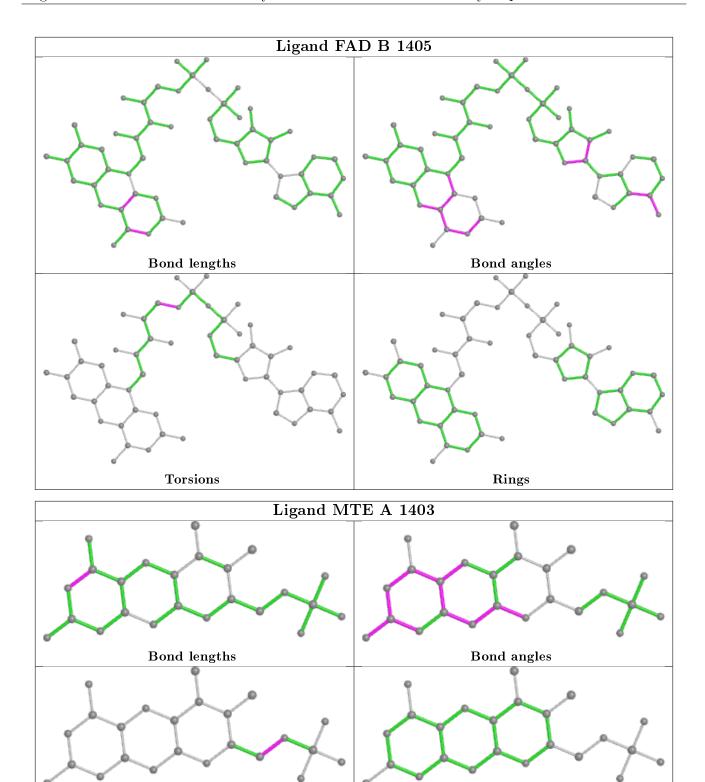
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1410	RAL	1	0
2	A	1401	FES	1	0
7	В	1408	RAL	1	0

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.





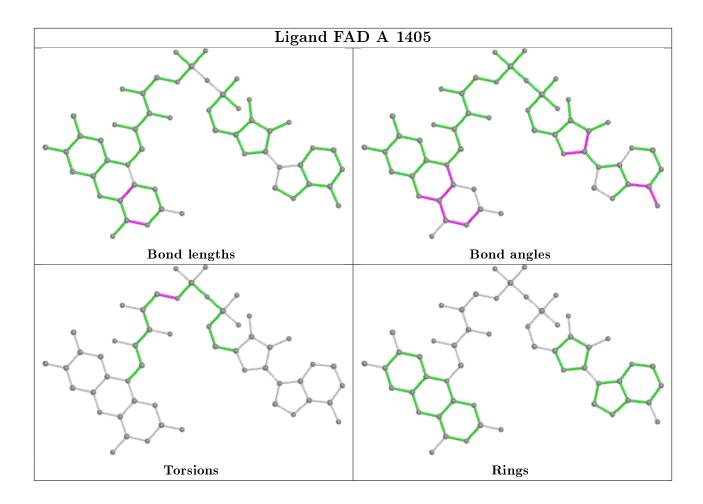




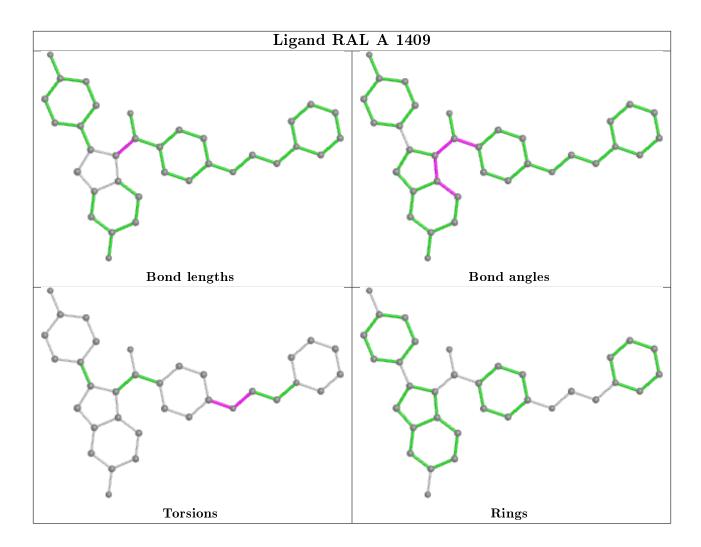


Torsions

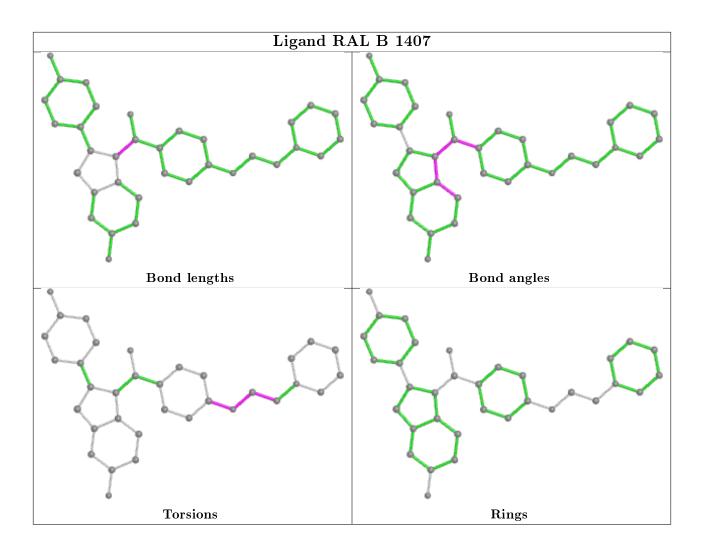
Rings



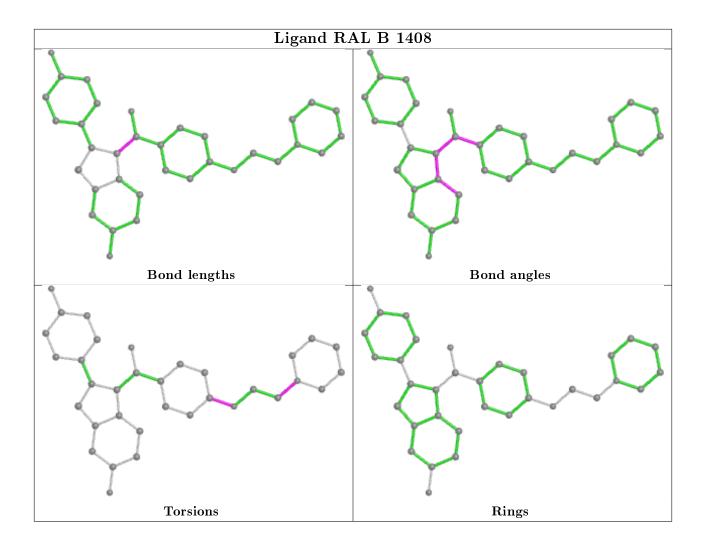












5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

