



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 05:46 AM EDT

PDB ID : 1JV7
Title : BACTERIORHODOPSIN O-LIKE INTERMEDIATE STATE OF THE D85S
MUTANT AT 2.25 ANGSTROM RESOLUTION
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Lanyi, J.K.; Glaeser, R.M.; Luecke, H.
Deposited on : 2001-08-28
Resolution : 2.25 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 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) : 2.23.2

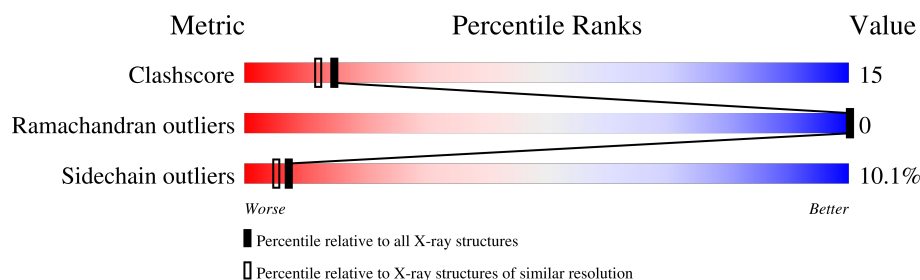
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)

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	249	

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
3	LI1	A	704	X	-	-	-
3	LI1	A	707	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1823 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.

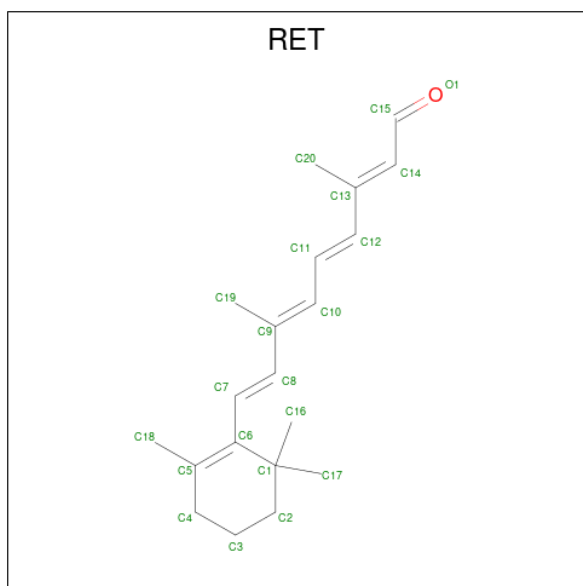
- Molecule 1 is a protein called Bacteriorhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1629	1099	246	276	8			

There is a discrepancy between the modelled and reference sequences:

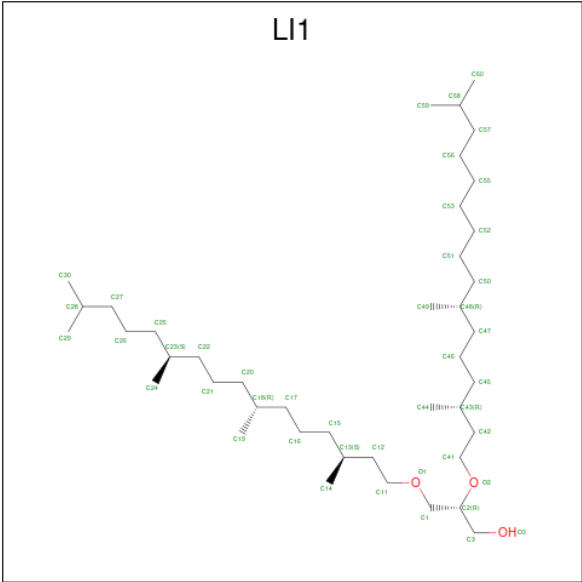
Chain	Residue	Modelled	Actual	Comment	Reference
A	85	SER	ASP	engineered mutation	UNP P02945

- Molecule 2 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			20	20		

- Molecule 3 is 1-[2,6,10,14-TETRAMETHYL-HEXADECAN-16-YL]-2-[2,10,14-TRIMETHYLHEXADECAN-16-YL]GLYCEROL (three-letter code: LI1) (formula: $C_{42}H_{86}O_3$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	0	0
			20	20		
3	A	1	Total	C	0	0
			16	16		
3	A	1	Total	C	0	0
			8	8		
3	A	1	Total	C	0	0
			32	29	3	
3	A	1	Total	C	0	0
			21	20	1	
3	A	1	Total	C	0	0
			11	11		
3	A	1	Total	C	0	0
			12	11	1	
3	A	1	Total	C	0	0
			12	11	1	
3	A	1	Total	C	0	0
			9	9		

- Molecule 4 is water.

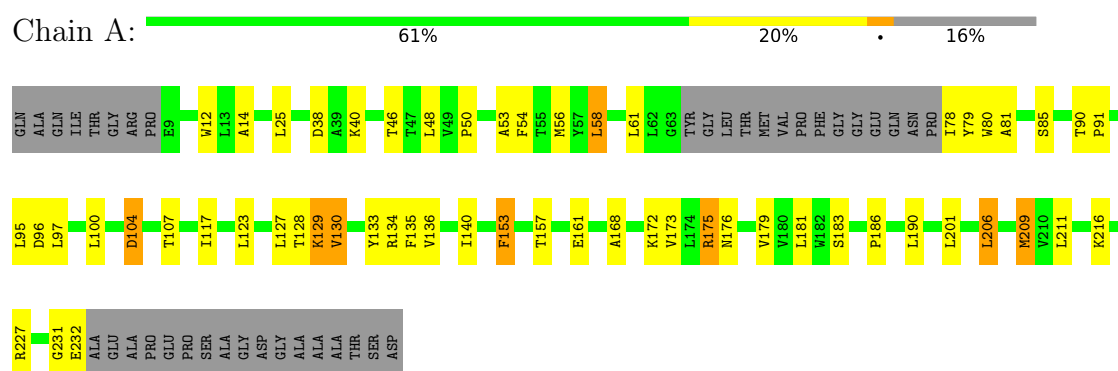
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total	O	0	0
			33	33		

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: Bacteriorhodopsin



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	51.80Å 121.30Å 85.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.25	Depositor
% Data completeness (in resolution range)	(Not available) (12.00-2.25)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.213 , 0.244	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1823	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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: LI1, RET

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	0.44	0/1671	0.57	0/2280

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	1629	0	1692	55	0
2	A	20	0	27	3	0
3	A	141	0	232	13	0
4	A	33	0	0	1	0
All	All	1823	0	1951	57	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 15.

All (57) 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:40:LYS:HA	1:A:40:LYS:HE2	1.53	0.90
1:A:130:VAL:CG2	1:A:133:TYR:HD1	1.92	0.83
1:A:129:LYS:HD3	1:A:129:LYS:H	1.53	0.74
1:A:129:LYS:HD3	1:A:129:LYS:N	2.04	0.72
1:A:90:THR:OG1	1:A:91:PRO:HD3	1.93	0.68
1:A:78:ILE:HG13	1:A:79:TYR:H	1.58	0.68
1:A:129:LYS:H	1:A:129:LYS:CD	2.05	0.67
1:A:56:MET:HG3	1:A:85:SER:HB3	1.75	0.66
1:A:130:VAL:HG21	1:A:133:TYR:HD1	1.62	0.65
1:A:186:PRO:O	1:A:190:LEU:HG	1.97	0.65
1:A:153:PHE:CE1	1:A:175:ARG:HD3	2.33	0.64
1:A:130:VAL:HG21	1:A:133:TYR:CD1	2.32	0.64
1:A:176:ASN:HD22	3:A:705:LI1:H142	1.64	0.61
1:A:53:ALA:HB2	1:A:216:LYS:HE3	1.82	0.61
1:A:58:LEU:HD13	3:A:704:LI1:H552	1.84	0.60
1:A:130:VAL:CG2	1:A:133:TYR:CD1	2.81	0.59
1:A:117:ILE:HD13	3:A:702:LI1:H472	1.84	0.58
1:A:12:TRP:CE2	1:A:206:LEU:HG	2.39	0.58
1:A:130:VAL:HG22	1:A:133:TYR:HD1	1.64	0.58
1:A:135:PHE:HE2	3:A:708:LI1:H193	1.70	0.57
1:A:153:PHE:HD1	1:A:179:VAL:HG21	1.71	0.56
1:A:173:VAL:HA	3:A:705:LI1:H141	1.90	0.54
1:A:14:ALA:HA	1:A:61:LEU:HD11	1.90	0.53
1:A:231:GLY:O	1:A:232:GLU:HB2	2.09	0.53
1:A:176:ASN:ND2	3:A:705:LI1:H142	2.25	0.52
1:A:123:LEU:C	1:A:123:LEU:HD13	2.30	0.51
1:A:128:THR:HG23	1:A:134:ARG:HB2	1.91	0.51
3:A:705:LI1:H28	3:A:706:LI1:H193	1.91	0.51
1:A:80:TRP:HB2	3:A:704:LI1:O3	2.12	0.49
1:A:153:PHE:CD1	1:A:179:VAL:HG21	2.48	0.49
1:A:181:LEU:HD23	3:A:705:LI1:H272	1.94	0.49
1:A:56:MET:SD	3:A:704:LI1:H172	2.53	0.49
1:A:186:PRO:HG3	2:A:301:RET:C18	2.42	0.48
1:A:209:MET:HE2	1:A:209:MET:O	2.13	0.48
1:A:40:LYS:HA	1:A:40:LYS:CE	2.36	0.48
1:A:201:LEU:O	1:A:201:LEU:HD13	2.14	0.48
1:A:183:SER:O	1:A:186:PRO:HD2	2.14	0.47
1:A:104:ASP:OD1	1:A:107:THR:HG23	2.15	0.47
1:A:123:LEU:O	1:A:127:LEU:HG	2.15	0.47
1:A:136:VAL:O	1:A:140:ILE:HG13	2.15	0.47
1:A:168:ALA:O	1:A:172:LYS:HG3	2.16	0.46
1:A:186:PRO:HG3	2:A:301:RET:H183	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ALA:HA	3:A:704:LI1:H12	1.99	0.45
1:A:130:VAL:HG22	1:A:133:TYR:H	1.83	0.44
1:A:79:TYR:CE1	1:A:201:LEU:HD11	2.53	0.43
1:A:181:LEU:CD2	3:A:705:LI1:H272	2.49	0.43
1:A:40:LYS:HE2	1:A:40:LYS:CA	2.35	0.43
1:A:46:THR:HG23	4:A:502:HOH:O	2.19	0.42
1:A:175:ARG:O	1:A:179:VAL:HG23	2.20	0.42
1:A:157:THR:O	1:A:161:GLU:HG3	2.20	0.41
1:A:12:TRP:HA	1:A:12:TRP:HE3	1.85	0.41
1:A:54:PHE:CZ	1:A:58:LEU:HD12	2.56	0.41
1:A:12:TRP:HA	1:A:12:TRP:CE3	2.56	0.41
1:A:56:MET:CE	3:A:704:LI1:H172	2.50	0.41
2:A:301:RET:H7	2:A:301:RET:H181	1.93	0.40
1:A:46:THR:O	1:A:50:PRO:HD2	2.21	0.40
1:A:56:MET:CE	1:A:56:MET:HA	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	206/249 (83%)	204 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	169/195 (87%)	152 (90%)	17 (10%)	7 5

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	38	ASP
1	A	48	LEU
1	A	58	LEU
1	A	95	LEU
1	A	96	ASP
1	A	97	LEU
1	A	100	LEU
1	A	104	ASP
1	A	129	LYS
1	A	130	VAL
1	A	153	PHE
1	A	175	ARG
1	A	206	LEU
1	A	209	MET
1	A	211	LEU
1	A	227	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

10 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$
3	LI1	A	706	-	10,10,44	0.80	0	11,11,51	0.70	0
3	LI1	A	703	-	7,7,44	0.94	0	6,6,51	0.99	0
3	LI1	A	701	-	19,19,44	1.14	1 (5%)	22,22,51	1.02	2 (9%)
3	LI1	A	705	-	20,20,44	1.18	1 (5%)	22,23,51	1.00	1 (4%)
2	RET	A	301	1	20,20,21	2.05	4 (20%)	27,27,28	1.15	3 (11%)
3	LI1	A	704	-	31,31,44	1.34	5 (16%)	32,32,51	1.11	2 (6%)
3	LI1	A	708	-	11,11,44	0.99	0	11,12,51	0.78	0
3	LI1	A	707	-	11,11,44	1.31	1 (9%)	10,11,51	1.13	0
3	LI1	A	709	-	8,8,44	0.70	0	8,8,51	0.70	0
3	LI1	A	702	-	15,15,44	1.00	0	14,14,51	0.86	0

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
3	LI1	A	706	-	-	3/10/10/49	-
3	LI1	A	703	-	-	2/5/5/49	-
3	LI1	A	701	-	-	10/20/20/49	-
3	LI1	A	705	-	-	4/21/21/49	-
2	RET	A	301	1	-	0/13/30/31	0/1/1/1
3	LI1	A	704	-	1/1/2/8	14/31/31/49	-
3	LI1	A	708	-	-	3/11/11/49	-
3	LI1	A	707	-	1/1/1/8	2/10/10/49	-
3	LI1	A	709	-	-	2/6/6/49	-
3	LI1	A	702	-	-	8/13/13/49	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	RET	C14-C13	5.81	1.38	1.33
2	A	301	RET	C1-C6	4.70	1.60	1.53
3	A	704	LI1	O2-C2	2.86	1.51	1.43
2	A	301	RET	C2-C3	-2.45	1.46	1.52
3	A	707	LI1	C42-C41	2.32	1.59	1.51
3	A	705	LI1	C12-C11	2.32	1.59	1.51
2	A	301	RET	C15-C14	-2.20	1.41	1.49
3	A	701	LI1	C16-C15	2.20	1.61	1.52
3	A	704	LI1	C3-C2	2.19	1.56	1.51
3	A	704	LI1	O2-C41	2.10	1.48	1.43
3	A	704	LI1	O3-C3	2.07	1.51	1.42
3	A	704	LI1	C42-C41	2.02	1.59	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	704	LI1	C41-O2-C2	3.63	123.74	115.40
3	A	701	LI1	C16-C17-C18	2.64	124.44	115.92
3	A	705	LI1	C16-C17-C18	2.50	123.99	115.92
3	A	704	LI1	O3-C3-C2	2.25	117.76	111.78
2	A	301	RET	C8-C7-C6	2.09	133.07	127.20
2	A	301	RET	C1-C6-C5	-2.07	119.69	122.61
2	A	301	RET	C7-C8-C9	2.07	129.37	126.23
3	A	701	LI1	C16-C15-C13	2.01	122.42	115.92

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	704	LI1	C2
3	A	707	LI1	C43

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	LI1	C24-C23-C25-C26
3	A	706	LI1	C15-C16-C17-C18
3	A	702	LI1	C43-C45-C46-C47
3	A	701	LI1	C26-C27-C28-C30
3	A	701	LI1	C26-C27-C28-C29
3	A	709	LI1	C12-C13-C15-C16
3	A	704	LI1	O2-C41-C42-C43

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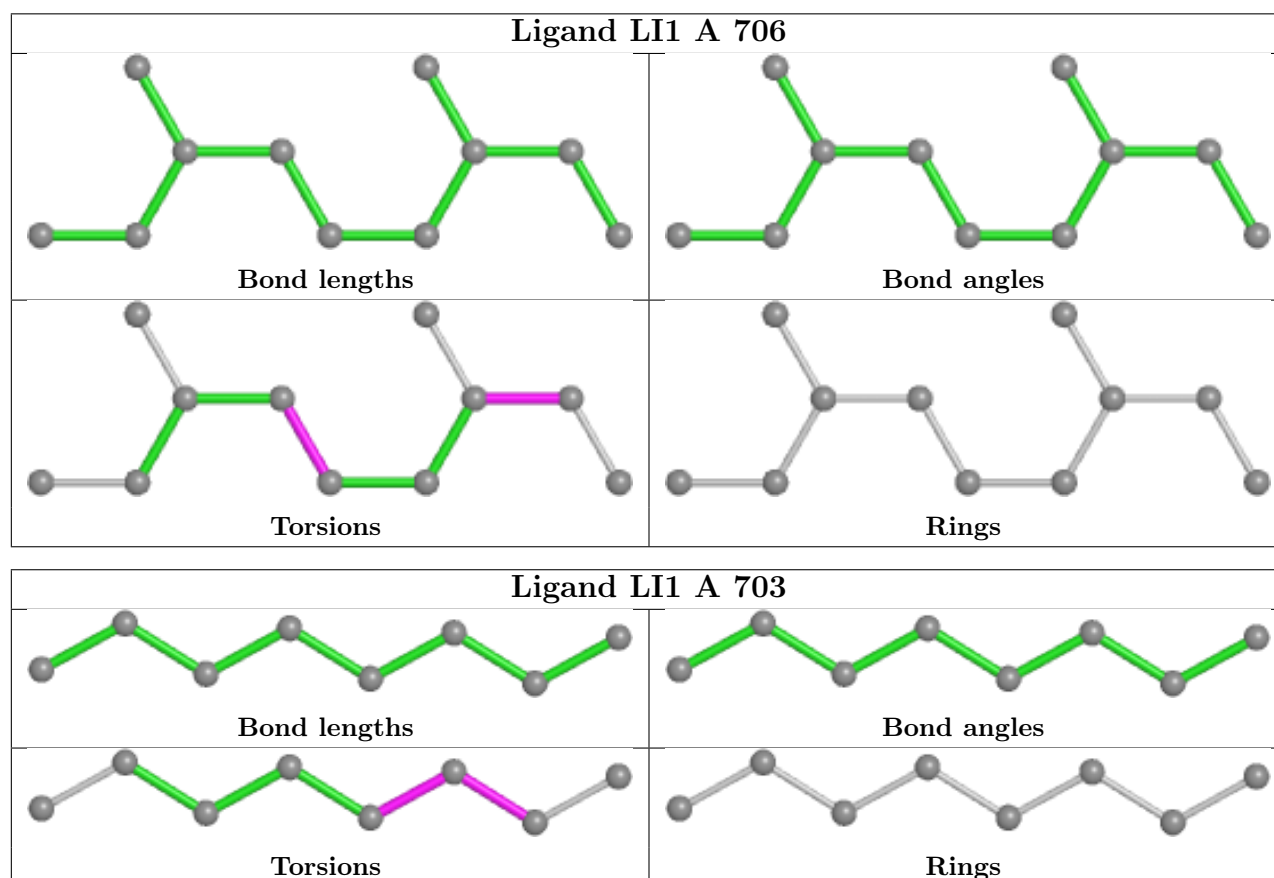
Mol	Chain	Res	Type	Atoms
3	A	704	LI1	C42-C41-O2-C2
3	A	704	LI1	C47-C48-C50-C51
3	A	704	LI1	C50-C51-C52-C53
3	A	704	LI1	C56-C57-C58-C59
3	A	704	LI1	C12-C13-C15-C16
3	A	704	LI1	C56-C57-C58-C60
3	A	709	LI1	C14-C13-C15-C16
3	A	702	LI1	C45-C46-C47-C48
3	A	704	LI1	C43-C45-C46-C47
3	A	701	LI1	C18-C20-C21-C22
3	A	704	LI1	C45-C46-C47-C48
3	A	702	LI1	C50-C51-C52-C53
3	A	701	LI1	C23-C25-C26-C27
3	A	702	LI1	C52-C53-C55-C56
3	A	703	LI1	C45-C46-C47-C48
3	A	704	LI1	C42-C43-C45-C46
3	A	702	LI1	C47-C48-C50-C51
3	A	704	LI1	C41-C42-C43-C45
3	A	701	LI1	C20-C21-C22-C23
3	A	703	LI1	C43-C45-C46-C47
3	A	704	LI1	C48-C50-C51-C52
3	A	701	LI1	C22-C23-C25-C26
3	A	705	LI1	O1-C11-C12-C13
3	A	708	LI1	C14-C13-C15-C16
3	A	708	LI1	C15-C16-C17-C18
3	A	701	LI1	C11-C12-C13-C14
3	A	701	LI1	C11-C12-C13-C15
3	A	706	LI1	C11-C12-C13-C15
3	A	704	LI1	C52-C53-C55-C56
3	A	705	LI1	C13-C15-C16-C17
3	A	706	LI1	C11-C12-C13-C14
3	A	702	LI1	C51-C52-C53-C55
3	A	708	LI1	C11-C12-C13-C15
3	A	702	LI1	C56-C57-C58-C59
3	A	702	LI1	C41-C42-C43-C45
3	A	705	LI1	C15-C16-C17-C18
3	A	707	LI1	C44-C43-C45-C46
3	A	705	LI1	C20-C21-C22-C23
3	A	704	LI1	C2-C1-O1-C11
3	A	701	LI1	C21-C22-C23-C25
3	A	707	LI1	C42-C43-C45-C46

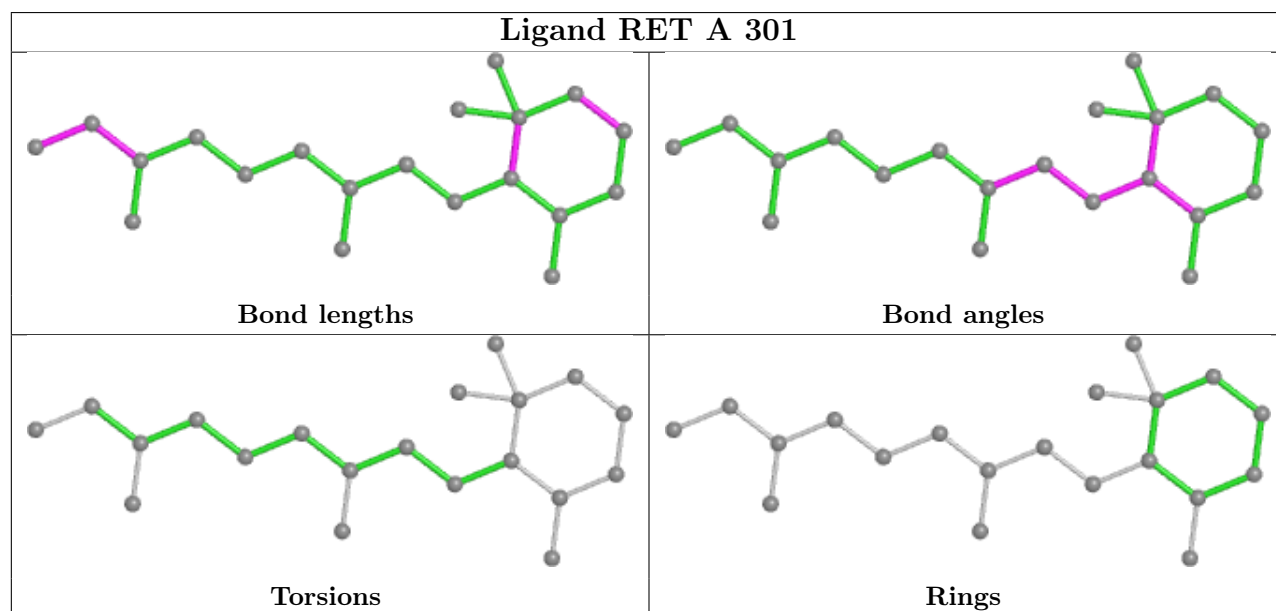
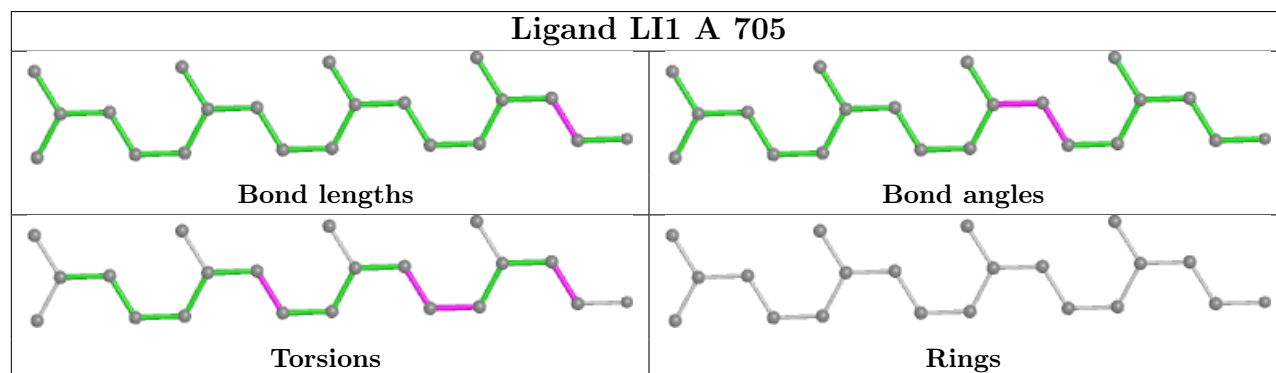
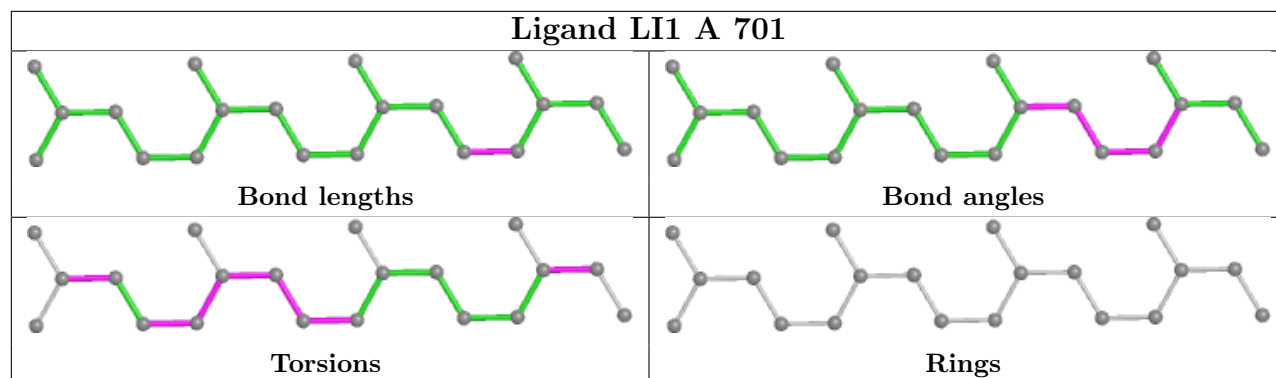
There are no ring outliers.

6 monomers are involved in 16 short contacts:

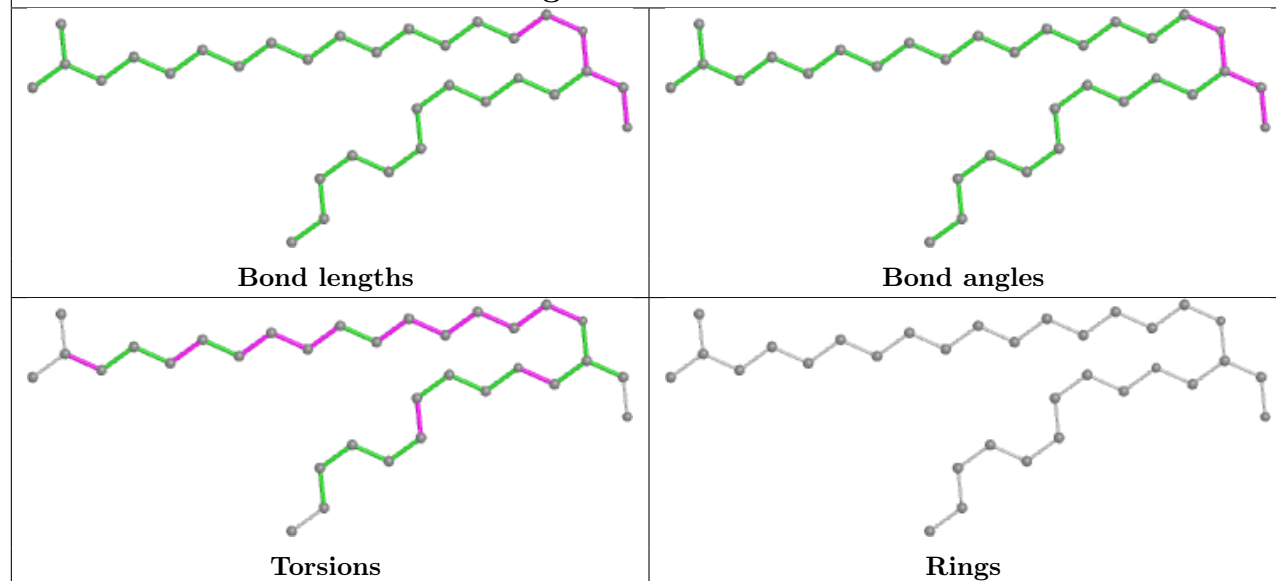
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	706	LI1	1	0
3	A	705	LI1	6	0
2	A	301	RET	3	0
3	A	704	LI1	5	0
3	A	708	LI1	1	0
3	A	702	LI1	1	0

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 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.

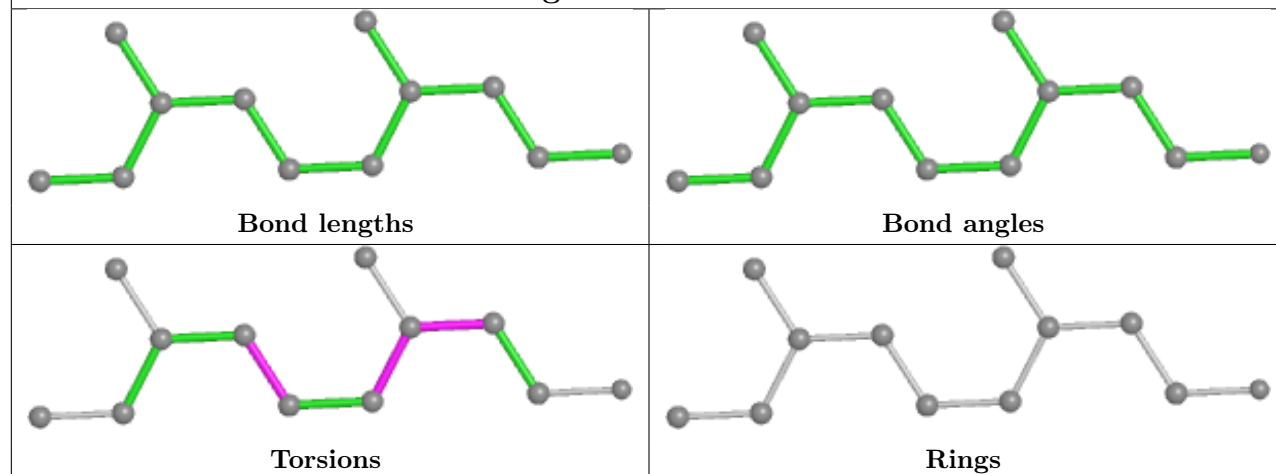




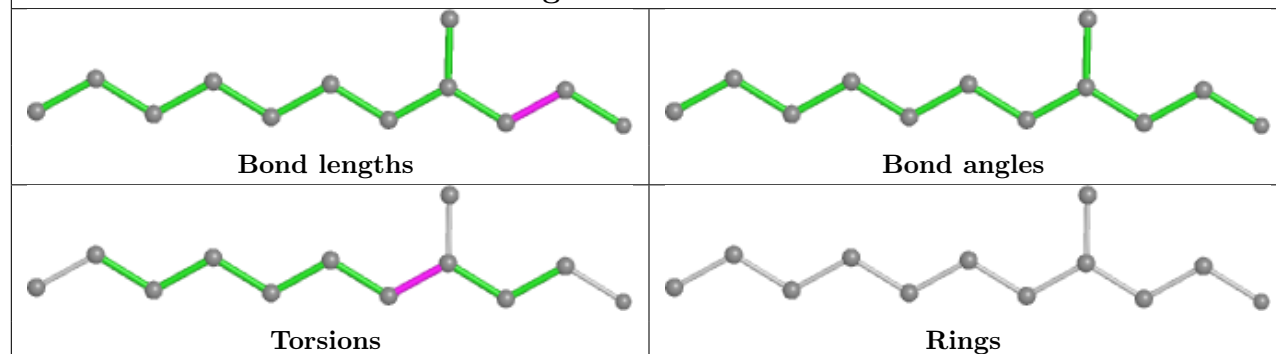
Ligand LI1 A 704

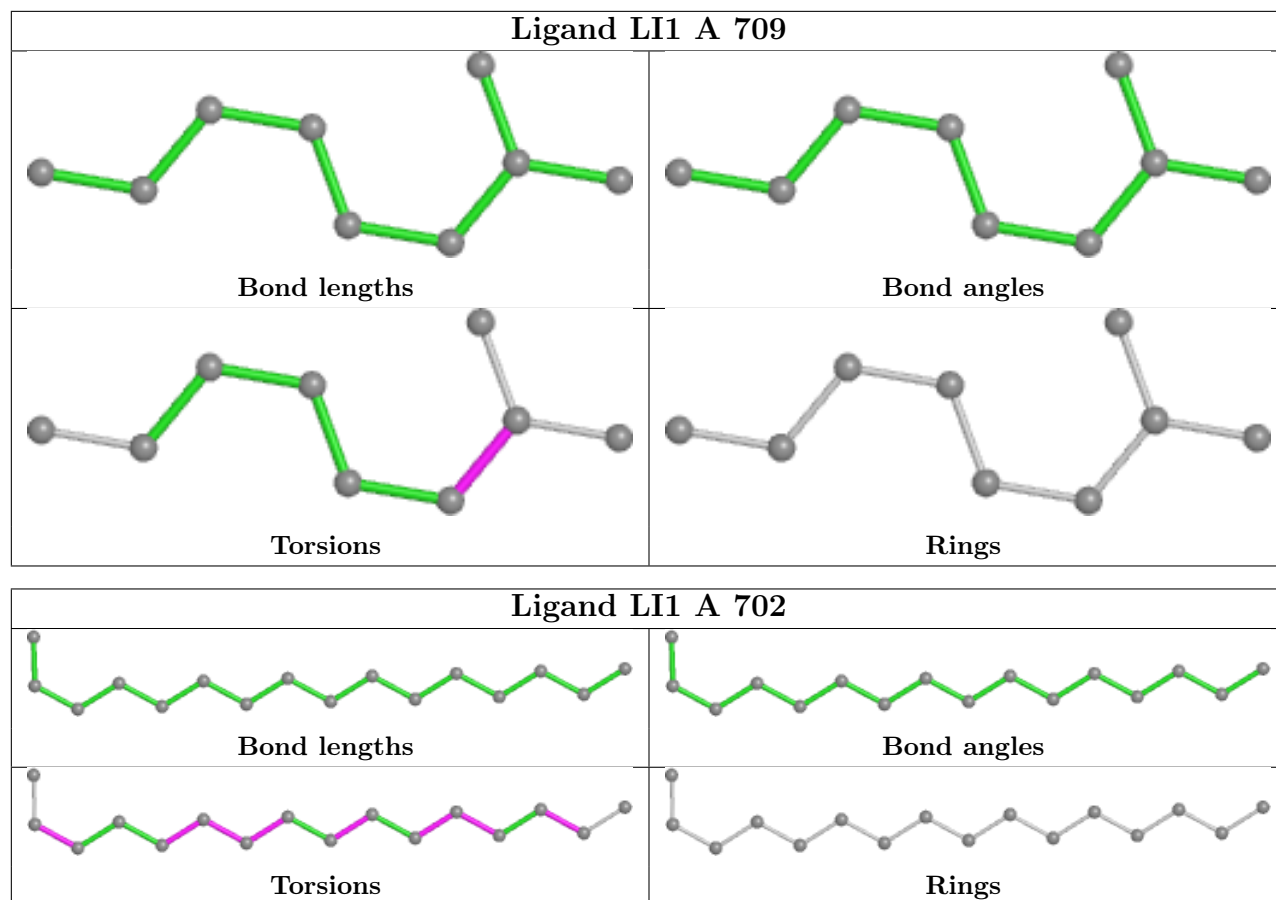


Ligand LI1 A 708



Ligand LI1 A 707





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.