



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:49 PM UTC

PDB ID : 1EPB / pdb_00001epb
Title : STRUCTURE OF THE EPIDIDYMAL RETINOIC ACID-BINDING PROTEIN AT 2.1 ANGSTROMS RESOLUTION
Authors : Newcomer, M.E.
Deposited on : 1993-06-15
Resolution : 2.20 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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

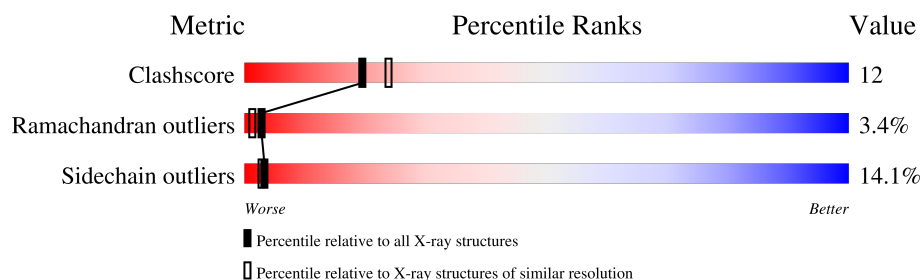
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	164	 57% 34% 5% ••
1	B	164	 53% 35% 10% •

2 Entry composition [i](#)

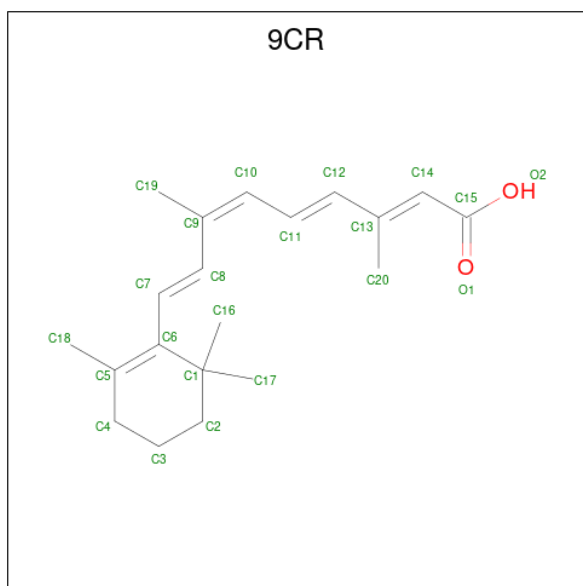
There are 3 unique types of molecules in this entry. The entry contains 2587 atoms, of which 42 are hydrogens and 0 are deuteriums.

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 EPIDIDYMAL RETINOIC ACID-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	0	0	9
			1201	773	190	233	5			
1	B	164	Total	C	N	O	S	0	0	9
			1228	789	194	240	5			

- Molecule 2 is (9cis)-retinoic acid (CCD ID: 9CR) (formula: $C_{20}H_{28}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			43	20	21	2		
2	B	1	Total	C	H	O	0	0
			43	20	21	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total 38	O 38	0	0
3	B	34	Total 34	O 34	0	0

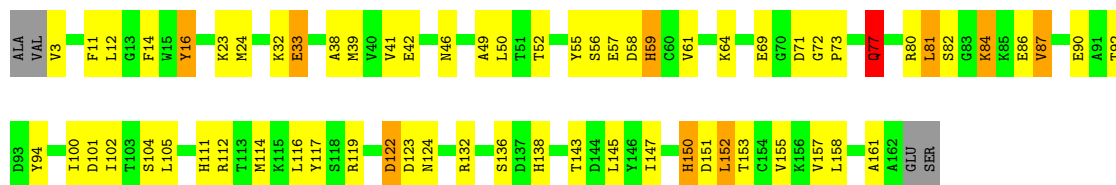
3 Residue-property plots [i](#)

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.

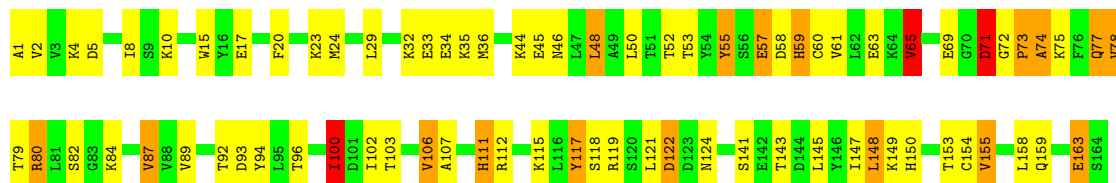
• Molecule 1: EPIDIDYMAL RETINOIC ACID-BINDING PROTEIN

Chain A: 



• Molecule 1: EPIDIDYMAL RETINOIC ACID-BINDING PROTEIN

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	39.80Å 58.89Å 66.65Å 90.00° 109.44° 90.00°	Depositor
Resolution (Å)	6.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.182 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2587	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: 9CR

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	1.13	7/1212 (0.6%)	1.83	24/1636 (1.5%)
1	B	1.17	7/1239 (0.6%)	1.86	33/1673 (2.0%)
All	All	1.15	14/2451 (0.6%)	1.85	57/3309 (1.7%)

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
1	A	0	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	HIS	CD2-NE2	-7.71	1.29	1.37
1	A	155	VAL	CA-CB	7.33	1.63	1.54
1	A	59	HIS	CD2-NE2	-6.52	1.30	1.37
1	B	59	HIS	CD2-NE2	-6.52	1.30	1.37
1	B	150	HIS	CD2-NE2	-6.50	1.30	1.37
1	A	111	HIS	CD2-NE2	-6.30	1.30	1.37
1	B	87	VAL	CA-CB	6.17	1.62	1.54
1	B	100	ILE	CA-CB	5.94	1.62	1.54
1	B	78	VAL	CA-CB	5.91	1.62	1.54
1	A	147	ILE	CA-CB	5.68	1.60	1.54
1	B	111	HIS	CD2-NE2	-5.49	1.31	1.37
1	A	59	HIS	CG-ND1	-5.35	1.32	1.38
1	A	150	HIS	CD2-NE2	-5.19	1.32	1.37
1	B	155	VAL	CA-CB	5.12	1.60	1.54

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	ASP	CA-CB-CG	10.10	122.70	112.60
1	B	122	ASP	CA-CB-CG	8.63	121.23	112.60
1	A	122	ASP	CA-CB-CG	8.44	121.04	112.60
1	B	71	ASP	CA-CB-CG	7.26	119.86	112.60
1	A	152	LEU	N-CA-C	6.95	121.78	113.16
1	A	150	HIS	CB-CG-CD2	-6.94	122.18	131.20
1	B	4	LYS	N-CA-C	6.74	120.81	112.59
1	B	159	GLN	OE1-CD-NE2	-6.60	116.00	122.60
1	B	77	GLN	OE1-CD-NE2	-6.59	116.01	122.60
1	A	81	LEU	O-C-N	6.58	131.35	122.59
1	B	71	ASP	CA-C-O	6.57	129.90	120.51
1	A	11	PHE	CA-CB-CG	-6.20	107.60	113.80
1	B	124	ASN	OD1-CG-ND2	-6.15	116.45	122.60
1	B	45	GLU	N-CA-C	-6.07	97.88	110.80
1	B	55	TYR	CA-CB-CG	6.03	124.76	113.90
1	A	77	GLN	OE1-CD-NE2	-6.02	116.58	122.60
1	A	69	GLU	CA-CB-CG	5.92	125.94	114.10
1	A	138	HIS	CB-CG-CD2	-5.91	123.52	131.20
1	B	103	THR	N-CA-C	-5.90	99.11	108.73
1	A	33	GLU	CA-CB-CG	-5.87	102.37	114.10
1	B	58	ASP	CA-CB-CG	5.80	118.41	112.60
1	B	57	GLU	CB-CG-CD	5.72	122.33	112.60
1	A	136	SER	N-CA-C	-5.69	105.16	111.36
1	B	63	GLU	O-C-N	-5.65	116.70	123.31
1	A	111	HIS	CB-CG-CD2	-5.63	123.89	131.20
1	B	115	LYS	CG-CD-CE	-5.50	98.64	111.30
1	A	123	ASP	N-CA-C	5.49	118.91	111.17
1	B	5	ASP	CA-C-O	5.48	126.90	121.20
1	B	124	ASN	CB-CG-ND2	5.48	124.62	116.40
1	B	59	HIS	CB-CG-CD2	-5.44	124.13	131.20
1	B	15	TRP	CE2-CD2-CG	-5.43	100.69	107.20
1	B	100	ILE	N-CA-CB	-5.42	101.19	111.21
1	A	49	ALA	N-CA-C	-5.41	100.89	109.76
1	A	77	GLN	CG-CD-NE2	5.39	124.49	116.40
1	B	96	THR	CA-CB-OG1	-5.39	101.51	109.60
1	A	150	HIS	CB-CG-ND1	5.36	130.74	122.70
1	B	111	HIS	CA-CB-CG	-5.34	108.46	113.80
1	B	77	GLN	CB-CG-CD	5.33	121.67	112.60
1	A	151	ASP	N-CA-C	-5.31	100.65	109.46
1	B	65	VAL	N-CA-CB	-5.27	102.26	110.96
1	A	143	THR	CA-CB-OG1	-5.26	101.70	109.60
1	B	117	TYR	CA-CB-CG	-5.25	104.45	113.90
1	B	44	LYS	CA-CB-CG	-5.24	103.63	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	VAL	N-CA-C	5.22	116.31	109.58
1	B	150	HIS	CB-CG-CD2	-5.22	124.42	131.20
1	B	148	LEU	N-CA-C	5.19	117.76	110.23
1	B	2	VAL	CA-C-O	-5.17	114.31	120.78
1	B	92	THR	CA-CB-OG1	-5.17	101.84	109.60
1	B	100	ILE	CB-CA-C	5.16	118.66	110.81
1	A	16	TYR	O-C-N	-5.14	117.46	123.27
1	A	46	ASN	CA-CB-CG	5.11	117.71	112.60
1	A	42	GLU	N-CA-C	-5.08	101.64	109.52
1	B	45	GLU	CA-CB-CG	5.07	124.23	114.10
1	B	118	SER	CA-C-O	5.06	126.93	121.06
1	B	163	GLU	CB-CG-CD	5.06	121.20	112.60
1	A	124	ASN	CA-CB-CG	5.05	117.65	112.60
1	A	92	THR	CA-CB-OG1	-5.03	102.05	109.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	72	GLY	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	1201	0	1184	25	0
1	B	1228	0	1214	29	0
2	A	22	21	27	4	0
2	B	22	21	27	4	0
3	A	38	0	0	0	0
3	B	34	0	0	2	0
All	All	2545	42	2452	56	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 12.

All (56) 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:23:LYS:C	1:A:24:MET:CA	2.45	0.88
1:B:23:LYS:C	1:B:24:MET:CA	2.52	0.83
1:A:39:MET:HE2	1:A:41:VAL:HG22	1.59	0.82
1:A:32:LYS:CA	1:A:33:GLU:N	2.46	0.79
1:A:39:MET:HG3	1:A:52:THR:HG22	1.67	0.74
1:A:117:TYR:CD2	2:A:165:9CR:H20	2.25	0.72
1:B:32:LYS:CA	1:B:33:GLU:N	2.54	0.70
1:B:117:TYR:CD1	2:B:165:9CR:H20	2.26	0.70
1:B:34:GLU:HB3	1:B:149:LYS:HB2	1.75	0.68
1:B:89:VAL:HG22	1:B:100:ILE:HD11	1.75	0.68
1:A:77:GLN:HB3	1:A:84:LYS:NZ	2.11	0.65
1:B:65:VAL:HG21	1:B:80:ARG:HH11	1.63	0.63
1:A:153:THR:O	1:A:157:VAL:HG23	1.98	0.63
1:A:150:HIS:HE1	3:B:179:HOH:O	1.82	0.63
1:B:82:SER:O	1:B:106:VAL:HA	1.98	0.62
1:B:53:THR:HA	1:B:61:VAL:O	1.99	0.61
1:B:1:ALA:HB1	1:B:74:ALA:HB3	1.82	0.61
1:A:39:MET:CE	1:A:50:LEU:HD22	2.33	0.58
1:B:36:MET:HG3	1:B:155:VAL:HG21	1.84	0.58
1:B:8:ILE:HG12	1:B:48:LEU:HD11	1.85	0.58
1:B:35:LYS:HE2	1:B:55:TYR:CD1	2.40	0.56
1:A:80:ARG:O	1:A:82:SER:N	2.41	0.54
1:B:117:TYR:CG	2:B:165:9CR:H20	2.44	0.52
1:A:77:GLN:HB3	1:A:84:LYS:HZ3	1.72	0.52
1:A:87:VAL:HA	1:A:101:ASP:O	2.10	0.51
1:B:80:ARG:NH2	2:B:165:9CR:H25	2.27	0.49
1:A:39:MET:HE1	1:A:50:LEU:HD22	1.95	0.47
2:A:165:9CR:H8	2:A:165:9CR:H16	1.97	0.47
1:A:14:PHE:HE1	1:A:16:TYR:CE1	2.33	0.46
2:B:165:9CR:H8	2:B:165:9CR:H16	1.97	0.46
1:B:65:VAL:HG21	1:B:80:ARG:HD3	1.98	0.46
1:A:80:ARG:NE	1:A:80:ARG:HA	2.31	0.46
1:B:79:THR:HG23	1:B:84:LYS:HG2	1.98	0.46
1:A:38:ALA:HB3	1:A:158:LEU:HD23	1.99	0.45
1:B:65:VAL:HG21	1:B:80:ARG:NH1	2.30	0.45
1:B:23:LYS:HB2	1:B:111:HIS:CE1	2.52	0.45
1:B:102:ILE:O	1:B:112:ARG:HA	2.17	0.44
1:B:74:ALA:HB1	1:B:89:VAL:HB	2.00	0.44
1:A:87:VAL:HG23	1:A:100:ILE:HG23	2.00	0.43
1:B:72:GLY:HA2	1:B:73:PRO:HD3	1.85	0.43
1:A:3:VAL:HG13	1:A:94:TYR:OH	2.18	0.43
1:B:147:ILE:HG12	3:B:181:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:LEU:HD11	2:A:165:9CR:H23	1.99	0.43
1:A:56:SER:O	1:A:59:HIS:ND1	2.52	0.43
1:A:102:ILE:HD13	2:A:165:9CR:C14	2.49	0.43
1:B:17:GLU:O	1:B:148:LEU:HD22	2.18	0.43
1:B:35:LYS:HE2	1:B:55:TYR:CE1	2.54	0.42
1:B:93:ASP:O	1:B:94:TYR:HB2	2.19	0.42
1:B:8:ILE:HD12	1:B:8:ILE:HA	1.93	0.42
1:B:60:CYS:CB	1:B:154:CYS:SG	3.07	0.42
1:A:90:GLU:HG3	1:A:114:MET:CE	2.50	0.41
1:A:132:ARG:NH1	1:A:145:LEU:HD12	2.35	0.41
1:A:39:MET:CE	1:A:41:VAL:HG22	2.41	0.41
1:B:20:PHE:HZ	1:B:29:LEU:CA	2.33	0.41
1:B:148:LEU:HD12	1:B:148:LEU:N	2.35	0.41
1:A:55:TYR:OH	1:A:58:ASP:HA	2.21	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	147/164 (90%)	133 (90%)	10 (7%)	4 (3%)	4	2
1	B	151/164 (92%)	135 (89%)	10 (7%)	6 (4%)	2	1
All	All	298/328 (91%)	268 (90%)	20 (7%)	10 (3%)	3	1

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	57	GLU
1	B	71	ASP
1	B	106	VAL
1	B	107	ALA

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Mol	Chain	Res	Type
1	A	57	GLU
1	A	73	PRO
1	A	81	LEU
1	B	74	ALA
1	A	161	ALA
1	B	73	PRO

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	130/139 (94%)	117 (90%)	13 (10%)	7	7
1	B	133/139 (96%)	109 (82%)	24 (18%)	2	1
All	All	263/278 (95%)	226 (86%)	37 (14%)	3	3

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	64	LYS
1	A	77	GLN
1	A	84	LYS
1	A	86	GLU
1	A	87	VAL
1	A	104	SER
1	A	105	LEU
1	A	112	ARG
1	A	116	LEU
1	A	119	ARG
1	A	122	ASP
1	A	152	LEU
1	B	10	LYS
1	B	46	ASN
1	B	48	LEU
1	B	50	LEU

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Mol	Chain	Res	Type
1	B	52	THR
1	B	59	HIS
1	B	65	VAL
1	B	69	GLU
1	B	71	ASP
1	B	75	LYS
1	B	77	GLN
1	B	78	VAL
1	B	80	ARG
1	B	87	VAL
1	B	100	ILE
1	B	119	ARG
1	B	121	LEU
1	B	122	ASP
1	B	141	SER
1	B	143	THR
1	B	145	LEU
1	B	153	THR
1	B	158	LEU
1	B	163	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	HIS
1	A	150	HIS
1	B	59	HIS
1	B	138	HIS
1	B	159	GLN

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 [i](#)

There are no oligosaccharides 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	$\# Z > 2$
2	9CR	A	165	-	22,22,22	1.14	2 (9%)	30,30,30	1.28	2 (6%)
2	9CR	B	165	-	22,22,22	1.14	2 (9%)	30,30,30	1.29	2 (6%)

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
2	9CR	A	165	-	-	4/15/32/32	0/1/1/1
2	9CR	B	165	-	-	4/15/32/32	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	165	9CR	O1-C15	3.88	1.32	1.23
2	A	165	9CR	O1-C15	3.85	1.32	1.23
2	A	165	9CR	O2-C15	-3.03	1.22	1.30
2	B	165	9CR	O2-C15	-3.01	1.22	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	165	9CR	O2-C15-C14	4.24	126.00	113.40
2	A	165	9CR	O2-C15-C14	4.23	125.98	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	165	9CR	O1-C15-C14	-3.90	112.07	124.02
2	B	165	9CR	O1-C15-C14	-3.90	112.08	124.02

There are no chirality outliers.

All (8) torsion outliers are listed below:

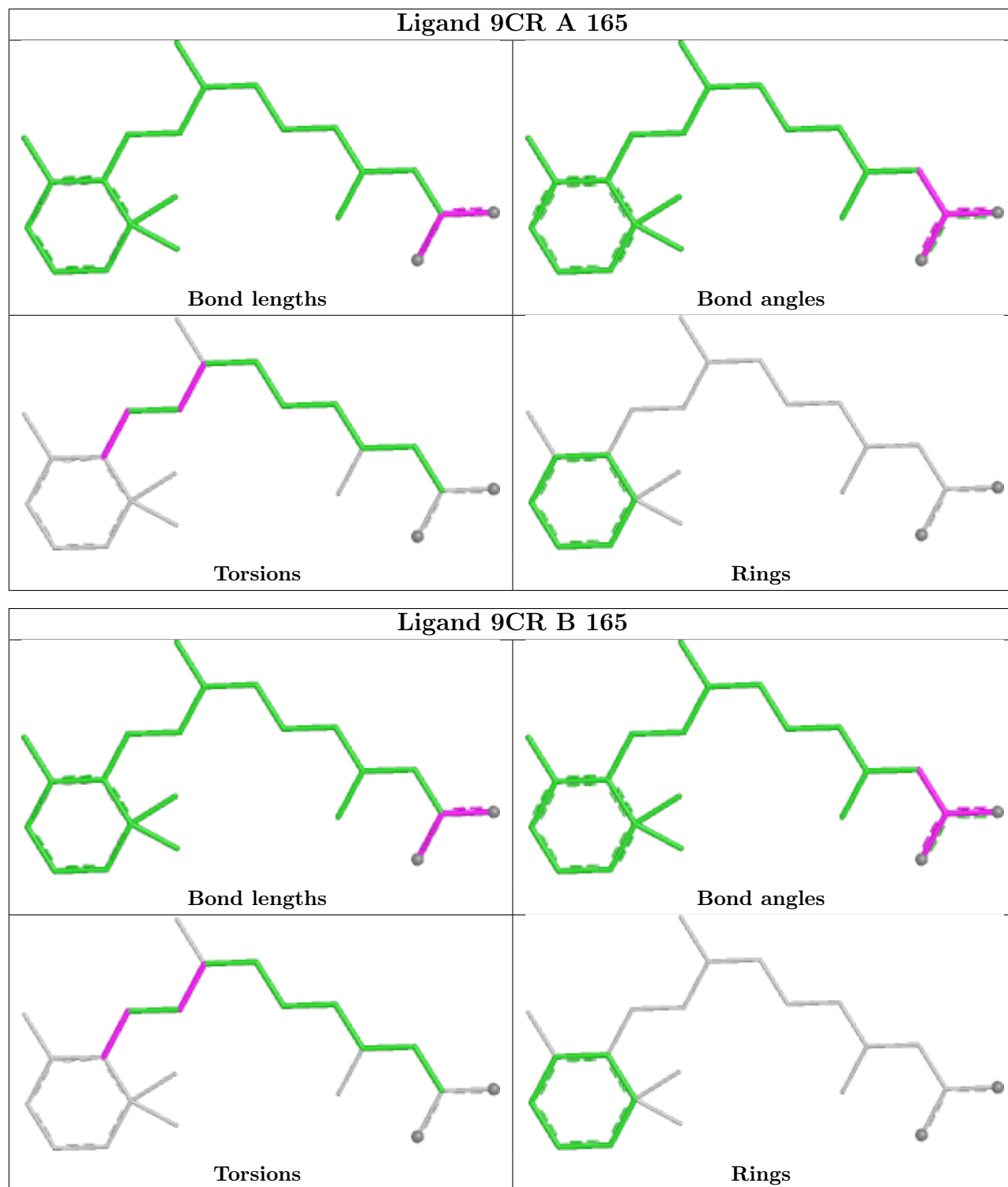
Mol	Chain	Res	Type	Atoms
2	A	165	9CR	C7-C8-C9-C19
2	B	165	9CR	C7-C8-C9-C19
2	A	165	9CR	C7-C8-C9-C10
2	B	165	9CR	C7-C8-C9-C10
2	A	165	9CR	C1-C6-C7-C8
2	A	165	9CR	C5-C6-C7-C8
2	B	165	9CR	C1-C6-C7-C8
2	B	165	9CR	C5-C6-C7-C8

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	165	9CR	4	0
2	B	165	9CR	4	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 ⓘ

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.