



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:27 PM UTC

PDB ID : 1TYR / pdb_00001tyr
Title : TRANSTHYRETIN COMPLEX WITH RETINOIC ACID
Authors : Zanotti, G.; D'Acunto, M.R.; Malpeli, G.; Folli, C.; Berni, R.
Deposited on : 1995-05-12
Resolution : 1.80 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

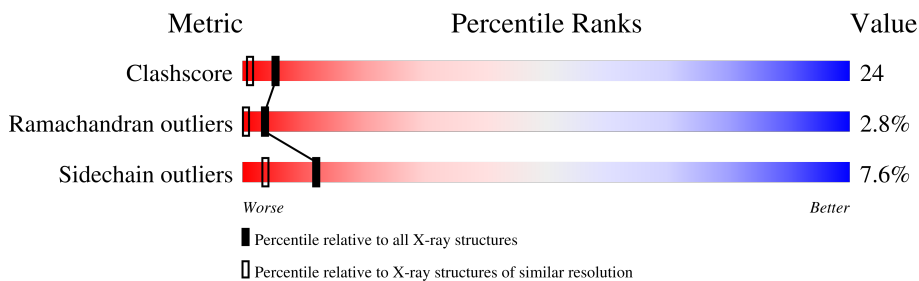
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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	127	
1	B	127	

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
2	9CR	A	131	-	-	X	-
2	9CR	B	130	-	-	X	-

2 Entry composition [i](#)

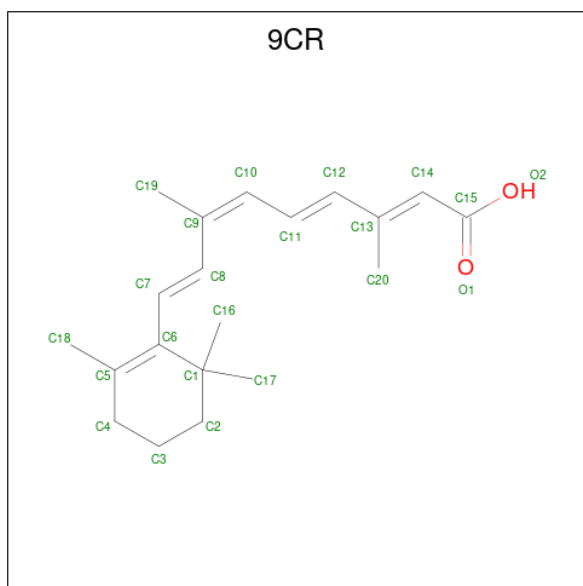
There are 3 unique types of molecules in this entry. The entry contains 2085 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRANSTHYRETIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	127	Total	C	N	O	S	0	0	0
			972	617	160	193	2			
1	B	127	Total	C	N	O	S	0	0	0
			972	617	160	193	2			

- Molecule 2 is (9cis)-retinoic acid (CCD ID: 9CR) (formula: C₂₀H₂₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			22	20	2		
2	B	1	Total	C	O	0	0
			22	20	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	53	Total 53	O 53	0	0
3	B	44	Total 44	O 44	0	0

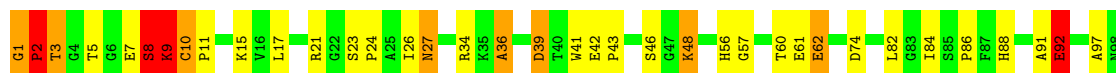
3 Residue-property plots

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.

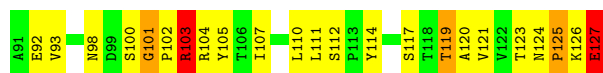
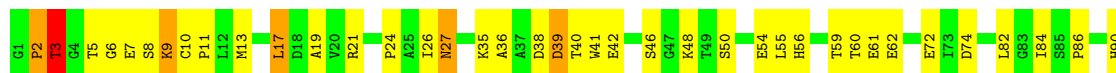
• Molecule 1: TRANSTHYRETIN

Chain A: 



• Molecule 1: TRANSTHYRETIN

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 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	43.80Å 86.22Å 65.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	9.00 – 1.80	Depositor
% Data completeness (in resolution range)	85.0 (9.00-1.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.196 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2085	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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: 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	6.90	1/997 (0.1%)	2.38	57/1357 (4.2%)
1	B	2.75	2/997 (0.2%)	2.27	42/1357 (3.1%)
All	All	5.25	3/1994 (0.2%)	2.33	99/2714 (3.6%)

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	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	GLU	C-OXT	213.82	5.51	1.23
1	B	127	GLU	C-OXT	75.33	2.74	1.23
1	B	7	GLU	CA-C	7.36	1.61	1.52

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	6	GLY	CA-C-N	9.90	135.66	122.30
1	B	6	GLY	C-N-CA	9.90	135.66	122.30
1	A	8	SER	N-CA-C	9.88	121.99	111.03
1	A	124	ASN	CA-CB-CG	-9.69	102.91	112.60
1	B	119	THR	CA-CB-OG1	-9.69	95.07	109.60
1	A	119	THR	OG1-CB-CG2	-8.96	91.38	109.30
1	B	24	PRO	N-CA-CB	8.93	111.64	103.33
1	B	7	GLU	N-CA-C	8.64	122.69	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	THR	CA-CB-OG1	8.48	122.31	109.60
1	A	27	ASN	OD1-CG-ND2	8.40	131.00	122.60
1	B	72	GLU	CB-CG-CD	-7.82	99.30	112.60
1	A	8	SER	CB-CA-C	-7.72	98.99	110.95
1	A	1	GLY	CA-C-N	7.66	129.41	119.84
1	A	1	GLY	C-N-CA	7.66	129.41	119.84
1	A	92	GLU	CB-CG-CD	7.61	125.54	112.60
1	A	39	ASP	N-CA-C	7.58	121.90	111.90
1	A	5	THR	N-CA-C	7.36	122.44	113.17
1	B	40	THR	CA-C-N	-7.15	112.00	122.65
1	B	40	THR	C-N-CA	-7.15	112.00	122.65
1	B	107	ILE	CB-CA-C	-6.81	101.02	110.96
1	B	111	LEU	N-CA-C	6.78	120.50	109.59
1	B	62	GLU	CB-CG-CD	-6.77	101.08	112.60
1	A	97	ALA	CA-C-N	6.69	131.64	122.07
1	A	97	ALA	C-N-CA	6.69	131.64	122.07
1	B	42	GLU	N-CA-CB	-6.69	96.60	110.45
1	A	123	THR	N-CA-CB	-6.64	99.73	111.08
1	B	7	GLU	CB-CA-C	6.55	121.16	110.22
1	B	39	ASP	CA-C-N	-6.54	111.35	122.67
1	B	39	ASP	C-N-CA	-6.54	111.35	122.67
1	A	26	ILE	CB-CA-C	-6.45	102.37	111.21
1	A	88	HIS	N-CA-C	6.40	119.96	110.48
1	A	41	TRP	N-CA-C	6.39	118.57	108.67
1	A	34	ARG	NE-CZ-NH2	-6.37	113.47	119.20
1	A	82	LEU	CB-CA-C	-6.36	99.42	110.17
1	A	15	LYS	CA-C-N	-6.35	114.29	123.06
1	A	15	LYS	C-N-CA	-6.35	114.29	123.06
1	B	10	CYS	CA-CB-SG	-6.34	99.81	114.40
1	A	36	ALA	N-CA-C	6.32	118.68	110.53
1	A	117	SER	N-CA-CB	-6.27	99.66	111.00
1	B	119	THR	CA-C-N	-6.27	113.54	122.94
1	B	119	THR	C-N-CA	-6.27	113.54	122.94
1	B	86	PRO	CB-CA-C	-6.18	101.37	111.56
1	B	98	ASN	CB-CA-C	-6.12	97.69	109.37
1	B	61	GLU	N-CA-C	6.07	118.69	111.71
1	A	116	TYR	N-CA-CB	6.04	122.75	111.52
1	A	9	LYS	N-CA-C	-6.00	98.03	110.80
1	B	17	LEU	CA-C-N	5.96	131.58	123.11
1	B	17	LEU	C-N-CA	5.96	131.58	123.11
1	A	86	PRO	N-CA-CB	-5.96	95.81	102.72
1	B	62	GLU	CA-CB-CG	-5.95	102.20	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	SER	O-C-N	-5.89	116.68	123.33
1	A	34	ARG	CG-CD-NE	-5.85	99.14	112.00
1	B	103	ARG	N-CA-C	5.81	120.39	113.12
1	A	56	HIS	CB-CA-C	-5.70	99.53	110.24
1	B	93	VAL	N-CA-C	-5.67	99.33	107.78
1	B	117	SER	N-CA-CB	-5.67	101.06	111.37
1	A	34	ARG	CA-C-N	-5.66	113.41	121.50
1	A	34	ARG	C-N-CA	-5.66	113.41	121.50
1	B	27	ASN	OD1-CG-ND2	5.65	128.25	122.60
1	B	127	GLU	N-CA-CB	5.63	120.08	110.50
1	B	7	GLU	CA-C-O	5.62	126.72	120.43
1	A	41	TRP	CB-CA-C	-5.61	101.41	110.77
1	A	124	ASN	CA-C-O	-5.61	115.17	119.32
1	A	102	PRO	CB-CA-C	-5.59	104.25	111.46
1	A	10	CYS	CA-CB-SG	-5.57	101.58	114.40
1	B	112	SER	O-C-N	-5.57	117.21	121.55
1	A	104	ARG	CA-C-N	-5.57	115.14	122.99
1	A	104	ARG	C-N-CA	-5.57	115.14	122.99
1	A	21	ARG	N-CA-CB	-5.55	102.49	110.65
1	B	48	LYS	O-C-N	-5.55	116.50	123.27
1	A	118	THR	O-C-N	-5.52	116.45	123.24
1	B	114	TYR	CA-C-N	-5.44	111.18	121.63
1	B	114	TYR	C-N-CA	-5.44	111.18	121.63
1	A	27	ASN	N-CA-CB	-5.40	104.09	112.30
1	A	48	LYS	CB-CG-CD	-5.39	98.90	111.30
1	A	2	PRO	CB-CA-C	5.38	120.43	111.56
1	A	62	GLU	CB-CG-CD	5.37	121.72	112.60
1	A	26	ILE	CB-CG1-CD1	-5.36	102.55	113.80
1	A	46	SER	N-CA-CB	5.35	119.85	111.56
1	B	105	TYR	CA-C-O	-5.29	114.64	120.30
1	B	46	SER	N-CA-CB	5.28	120.44	111.57
1	B	111	LEU	CB-CA-C	-5.27	99.90	109.38
1	A	60	THR	CA-CB-CG2	-5.25	101.58	110.50
1	B	19	ALA	N-CA-C	5.24	119.52	113.18
1	A	3	THR	N-CA-CB	-5.24	101.95	110.59
1	A	11	PRO	CB-CA-C	-5.11	104.22	111.68
1	A	91	ALA	N-CA-C	-5.10	101.09	109.40
1	A	99	ASP	CA-CB-CG	-5.09	107.51	112.60
1	B	102	PRO	N-CA-CB	5.07	110.11	103.42
1	B	72	GLU	N-CA-CB	-5.06	102.62	110.57
1	B	74	ASP	N-CA-CB	5.05	117.86	110.58
1	A	5	THR	CA-CB-OG1	5.02	117.13	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	HIS	CA-C-N	-5.01	112.10	121.07
1	A	56	HIS	C-N-CA	-5.01	112.10	121.07
1	A	5	THR	CB-CA-C	5.01	118.46	110.09
1	A	74	ASP	CA-C-N	-5.01	112.69	120.31
1	A	74	ASP	C-N-CA	-5.01	112.69	120.31
1	A	41	TRP	CA-C-O	5.01	126.26	120.60
1	A	43	PRO	CB-CA-C	-5.01	105.33	111.64

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	103	ARG	Sidechain

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	972	0	945	33	0
1	B	972	0	945	56	0
2	A	22	0	28	17	23
2	B	22	0	28	17	26
3	A	53	0	0	3	0
3	B	44	0	0	3	5
All	All	2085	0	1946	94	50

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 24.

All (94) 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:130:9CR:H9	2:B:130:9CR:H26	1.31	1.10
2:A:131:9CR:H9	2:A:131:9CR:H26	1.31	1.08
1:A:17:LEU:HD11	2:A:131:9CR:H26	1.39	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:9CR:H9	2:B:130:9CR:C20	1.89	1.02
2:A:131:9CR:H9	2:A:131:9CR:C20	1.89	1.01
1:B:17:LEU:HD11	2:B:130:9CR:H23	1.43	0.98
1:B:17:LEU:HD11	2:B:130:9CR:C19	1.93	0.98
1:B:104:ARG:HE	1:B:127:GLU:HA	1.26	0.97
1:B:13:MET:HB2	1:B:104:ARG:HH12	1.29	0.96
1:B:13:MET:HB2	1:B:104:ARG:NH1	1.83	0.92
1:A:108:ALA:HB3	2:A:131:9CR:H13	1.50	0.91
1:B:13:MET:HG3	1:B:104:ARG:HH22	1.34	0.90
1:A:119:THR:HG22	2:A:131:9CR:H14	1.61	0.82
1:A:119:THR:HG22	2:A:131:9CR:C16	2.10	0.82
1:B:127:GLU:OXT	2:B:130:9CR:C14	2.28	0.82
1:B:127:GLU:OXT	3:B:281:HOH:O	2.01	0.79
1:B:2:PRO:HD3	1:B:50:SER:HB3	1.63	0.78
1:A:115:SER:HB2	1:B:119:THR:HG23	1.66	0.77
1:A:119:THR:CG2	2:A:131:9CR:H14	2.14	0.77
1:B:82:LEU:HB3	1:B:84:ILE:HD12	1.67	0.77
1:B:127:GLU:OXT	2:B:130:9CR:O1	2.03	0.76
1:B:121:VAL:HG21	2:B:130:9CR:H25	1.67	0.75
1:B:17:LEU:HD12	2:B:130:9CR:H7	1.68	0.75
1:B:127:GLU:OXT	2:B:130:9CR:C15	2.35	0.74
1:B:2:PRO:CD	1:B:50:SER:HB3	2.17	0.74
2:B:130:9CR:C20	2:B:130:9CR:C10	2.65	0.74
1:B:124:ASN:H	1:B:125:PRO:HD2	1.53	0.74
1:B:110:LEU:HD22	2:B:130:9CR:H2	1.71	0.73
1:A:110:LEU:HB2	2:A:131:9CR:H18	1.71	0.72
1:B:2:PRO:O	1:B:3:THR:HB	1.90	0.71
1:B:103:ARG:HH11	1:B:103:ARG:HG3	1.55	0.70
1:A:108:ALA:CB	2:A:131:9CR:H13	2.21	0.69
1:B:104:ARG:NE	1:B:127:GLU:HA	2.06	0.68
1:B:17:LEU:CD1	2:B:130:9CR:H23	2.21	0.67
1:B:121:VAL:CG2	2:B:130:9CR:H25	2.24	0.67
1:A:92:GLU:OE1	1:A:92:GLU:N	2.26	0.66
1:B:17:LEU:HD11	2:B:130:9CR:H24	1.76	0.65
1:B:103:ARG:HG3	1:B:103:ARG:NH1	2.11	0.64
1:A:48:LYS:HE2	3:A:233:HOH:O	1.97	0.64
2:A:131:9CR:C20	2:A:131:9CR:C10	2.65	0.64
1:B:121:VAL:HG21	2:B:130:9CR:C14	2.30	0.61
1:B:36:ALA:O	1:B:39:ASP:N	2.31	0.60
1:A:7:GLU:HB3	1:A:57:GLY:HA2	1.83	0.60
1:B:13:MET:HG3	1:B:104:ARG:NH2	2.13	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:THR:HB	1:B:125:PRO:HD2	1.85	0.58
1:A:3:THR:OG1	1:A:62:GLU:HG3	2.04	0.58
1:A:17:LEU:CD1	2:A:131:9CR:H26	2.24	0.57
1:B:103:ARG:HH11	1:B:103:ARG:CG	2.17	0.56
1:A:17:LEU:HD11	2:A:131:9CR:C20	2.23	0.56
1:B:8:SER:OG	1:B:9:LYS:N	2.36	0.56
1:A:3:THR:HG22	3:A:268:HOH:O	2.06	0.55
1:A:117:SER:OG	2:A:131:9CR:H4	2.06	0.55
1:B:11:PRO:HG2	1:B:59:THR:HG23	1.87	0.54
1:B:13:MET:HB2	1:B:104:ARG:CZ	2.35	0.54
1:A:126:LYS:HA	1:A:127:GLU:OXT	2.07	0.54
1:B:104:ARG:HE	1:B:127:GLU:CA	2.09	0.53
1:B:21:ARG:NH2	3:B:238:HOH:O	2.42	0.53
1:A:119:THR:CB	2:A:131:9CR:H14	2.39	0.53
1:B:35:LYS:HB2	1:B:41:TRP:CZ3	2.44	0.52
1:A:126:LYS:HG3	1:A:127:GLU:OXT	2.10	0.51
1:B:17:LEU:CD1	2:B:130:9CR:C19	2.80	0.51
1:B:13:MET:CG	1:B:104:ARG:HH22	2.16	0.51
1:B:8:SER:CB	1:B:60:THR:HG22	2.41	0.51
1:A:84:ILE:HG23	3:A:225:HOH:O	2.11	0.50
1:B:56:HIS:HE1	3:B:277:HOH:O	1.93	0.50
1:B:90:HIS:CD2	1:B:92:GLU:HG3	2.46	0.50
1:A:8:SER:OG	1:A:9:LYS:N	2.42	0.49
1:A:109:ALA:C	2:A:131:9CR:H17	2.38	0.49
1:B:38:ASP:O	1:B:39:ASP:HB2	2.12	0.49
1:B:54:GLU:HB2	1:B:56:HIS:CE1	2.48	0.48
1:A:2:PRO:O	1:A:62:GLU:HG2	2.13	0.48
1:A:108:ALA:HB3	2:A:131:9CR:C16	2.33	0.48
1:B:82:LEU:HB3	1:B:84:ILE:CD1	2.41	0.47
1:A:23:SER:HB2	1:A:24:PRO:HD2	1.96	0.47
1:B:124:ASN:N	1:B:125:PRO:HD2	2.25	0.47
1:A:124:ASN:OD1	1:A:125:PRO:HD2	2.14	0.47
1:B:124:ASN:H	1:B:125:PRO:CD	2.24	0.45
1:A:9:LYS:HB2	1:A:9:LYS:HE2	1.82	0.45
1:A:92:GLU:N	1:A:92:GLU:CD	2.74	0.44
1:B:101:GLY:O	1:B:103:ARG:NH1	2.51	0.44
1:A:7:GLU:HB2	1:A:10:CYS:SG	2.58	0.44
1:A:7:GLU:CB	1:A:10:CYS:SG	3.06	0.44
1:B:17:LEU:CD1	2:B:130:9CR:H7	2.42	0.43
1:A:119:THR:HG22	2:A:131:9CR:H13	1.93	0.43
1:B:8:SER:HG	1:B:9:LYS:H	1.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:THR:HA	1:B:56:HIS:O	2.18	0.42
1:B:59:THR:OG1	1:B:60:THR:N	2.51	0.42
1:B:2:PRO:HB2	1:B:3:THR:H	1.69	0.42
1:B:8:SER:HB2	1:B:60:THR:HG22	2.01	0.42
1:A:36:ALA:HB2	1:A:42:GLU:HG3	2.01	0.41
1:B:26:ILE:O	1:B:27:ASN:HB2	2.19	0.41
1:B:124:ASN:N	1:B:125:PRO:CD	2.80	0.41
1:B:119:THR:HG22	1:B:120:ALA:N	2.36	0.41
1:A:1:GLY:HA2	1:A:2:PRO:HD2	1.73	0.41

All (50) 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)
2:A:131:9CR:C9	2:A:131:9CR:C9[2_665]	0.39	1.81
2:B:130:9CR:C17	2:B:130:9CR:C18[2_665]	0.39	1.81
2:B:130:9CR:C8	2:B:130:9CR:C8[2_665]	0.46	1.74
2:B:130:9CR:C2	3:B:260:HOH:O[2_665]	0.61	1.59
2:B:130:9CR:C3	2:B:130:9CR:C4[2_665]	0.71	1.49
2:A:131:9CR:C1	2:A:131:9CR:C18[2_665]	0.80	1.40
2:A:131:9CR:C4	2:A:131:9CR:C4[2_665]	0.81	1.39
2:A:131:9CR:C3	2:A:131:9CR:C4[2_665]	0.84	1.36
2:A:131:9CR:C10	2:A:131:9CR:C19[2_665]	0.85	1.35
2:B:130:9CR:C9	2:B:130:9CR:C9[2_665]	0.97	1.23
2:A:131:9CR:C17	2:A:131:9CR:C18[2_665]	1.09	1.11
2:A:131:9CR:C9	2:A:131:9CR:C10[2_665]	1.12	1.08
2:B:130:9CR:C3	3:B:260:HOH:O[2_665]	1.19	1.01
2:B:130:9CR:C19	3:B:274:HOH:O[2_665]	1.23	0.97
2:A:131:9CR:C5	2:A:131:9CR:C5[2_665]	1.25	0.95
2:A:131:9CR:C5	2:A:131:9CR:C6[2_665]	1.26	0.94
2:B:130:9CR:C10	2:B:130:9CR:C19[2_665]	1.36	0.84
2:B:130:9CR:C1	2:B:130:9CR:C18[2_665]	1.37	0.83
2:B:130:9CR:C1	3:B:260:HOH:O[2_665]	1.38	0.82
2:A:131:9CR:C8	2:A:131:9CR:C9[2_665]	1.41	0.79
2:B:130:9CR:C3	2:B:130:9CR:C3[2_665]	1.43	0.77
2:B:130:9CR:C9	2:B:130:9CR:C10[2_665]	1.45	0.75
2:A:131:9CR:C7	2:A:131:9CR:C8[2_665]	1.51	0.69
2:B:130:9CR:C7	2:B:130:9CR:C8[2_665]	1.56	0.64
2:B:130:9CR:C8	2:B:130:9CR:C9[2_665]	1.58	0.62
2:B:130:9CR:C6	2:B:130:9CR:C6[2_665]	1.58	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:131:9CR:C6	2:A:131:9CR:C6[2_665]	1.61	0.59
2:A:131:9CR:C6	2:A:131:9CR:C18[2_665]	1.62	0.58
3:B:274:HOH:O	3:B:274:HOH:O[2_665]	1.69	0.51
2:B:130:9CR:C1	2:B:130:9CR:C5[2_665]	1.70	0.50
2:B:130:9CR:C5	2:B:130:9CR:C6[2_665]	1.74	0.46
2:B:130:9CR:C4	2:B:130:9CR:C4[2_665]	1.74	0.46
2:B:130:9CR:C2	2:B:130:9CR:C4[2_665]	1.75	0.45
2:A:131:9CR:C4	2:A:131:9CR:C5[2_665]	1.82	0.38
2:A:131:9CR:C2	2:A:131:9CR:C18[2_665]	1.82	0.38
2:B:130:9CR:C5	2:B:130:9CR:C17[2_665]	1.82	0.38
2:A:131:9CR:C9	2:A:131:9CR:C19[2_665]	1.90	0.30
2:A:131:9CR:C1	2:A:131:9CR:C5[2_665]	1.90	0.30
2:A:131:9CR:C11	2:A:131:9CR:C19[2_665]	1.92	0.28
2:A:131:9CR:C7	2:A:131:9CR:C7[2_665]	1.94	0.26
2:A:131:9CR:C10	2:A:131:9CR:C10[2_665]	1.95	0.25
2:A:131:9CR:C3	2:A:131:9CR:C5[2_665]	1.95	0.25
2:A:131:9CR:C2	2:A:131:9CR:C4[2_665]	1.98	0.22
2:B:130:9CR:C3	2:B:130:9CR:C5[2_665]	2.01	0.19
2:B:130:9CR:C7	2:B:130:9CR:C7[2_665]	2.05	0.15
2:B:130:9CR:C2	2:B:130:9CR:C5[2_665]	2.12	0.08
2:B:130:9CR:C5	2:B:130:9CR:C5[2_665]	2.12	0.08
2:B:130:9CR:C2	2:B:130:9CR:C18[2_665]	2.17	0.03
2:A:131:9CR:C19	2:A:131:9CR:C20[2_665]	2.18	0.02
2:B:130:9CR:C9	2:B:130:9CR:C19[2_665]	2.18	0.02

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	125/127 (98%)	118 (94%)	4 (3%)	3 (2%)	4	1
1	B	125/127 (98%)	109 (87%)	12 (10%)	4 (3%)	3	0
All	All	250/254 (98%)	227 (91%)	16 (6%)	7 (3%)	4	0

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	PRO
1	A	126	LYS
1	B	2	PRO
1	B	5	THR
1	B	101	GLY
1	A	125	PRO
1	B	125	PRO

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	105/105 (100%)	96 (91%)	9 (9%)	10	3
1	B	105/105 (100%)	98 (93%)	7 (7%)	15	5
All	All	210/210 (100%)	194 (92%)	16 (8%)	12	4

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	9	LYS
1	A	27	ASN
1	A	39	ASP
1	A	61	GLU
1	A	92	GLU
1	A	100	SER
1	A	126	LYS
1	A	127	GLU
1	B	3	THR
1	B	9	LYS
1	B	55	LEU
1	B	100	SER
1	B	103	ARG
1	B	126	LYS
1	B	127	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	B	27	ASN
1	B	56	HIS
1	B	90	HIS

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 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	B	130	-	22,22,22	2.91	7 (31%)	30,30,30	3.46	5 (16%)
2	9CR	A	131	-	22,22,22	2.91	7 (31%)	30,30,30	3.46	6 (20%)

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	B	130	-	-	5/15/32/32	0/1/1/1
2	9CR	A	131	-	-	3/15/32/32	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	131	9CR	O1-C15	7.96	1.42	1.23
2	B	130	9CR	O1-C15	7.93	1.42	1.23
2	B	130	9CR	C1-C6	5.97	1.61	1.53
2	A	131	9CR	C1-C6	5.95	1.61	1.53
2	B	130	9CR	C8-C7	5.39	1.49	1.33
2	A	131	9CR	C8-C7	5.38	1.49	1.33
2	B	130	9CR	C2-C3	-3.64	1.44	1.52
2	A	131	9CR	C2-C3	-3.64	1.44	1.52
2	A	131	9CR	C20-C13	3.59	1.58	1.50
2	B	130	9CR	C20-C13	3.52	1.58	1.50
2	B	130	9CR	O2-C15	3.49	1.39	1.30
2	A	131	9CR	O2-C15	3.44	1.39	1.30
2	B	130	9CR	C5-C6	3.02	1.39	1.34
2	A	131	9CR	C5-C6	3.02	1.39	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	131	9CR	O2-C15-O1	-14.26	93.68	122.70
2	B	130	9CR	O2-C15-O1	-14.26	93.68	122.70
2	A	131	9CR	O2-C15-C14	9.95	142.99	113.40
2	B	130	9CR	O2-C15-C14	9.92	142.88	113.40
2	A	131	9CR	C15-C14-C13	-4.56	121.62	128.40
2	B	130	9CR	C15-C14-C13	-4.52	121.67	128.40
2	A	131	9CR	C7-C8-C9	3.77	131.81	126.23
2	B	130	9CR	C7-C8-C9	3.76	131.80	126.23
2	A	131	9CR	C18-C5-C6	2.23	126.92	124.48
2	B	130	9CR	C18-C5-C6	2.20	126.89	124.48
2	A	131	9CR	C19-C9-C10	2.01	126.07	122.82

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	131	9CR	C12-C13-C14-C15
2	A	131	9CR	C20-C13-C14-C15

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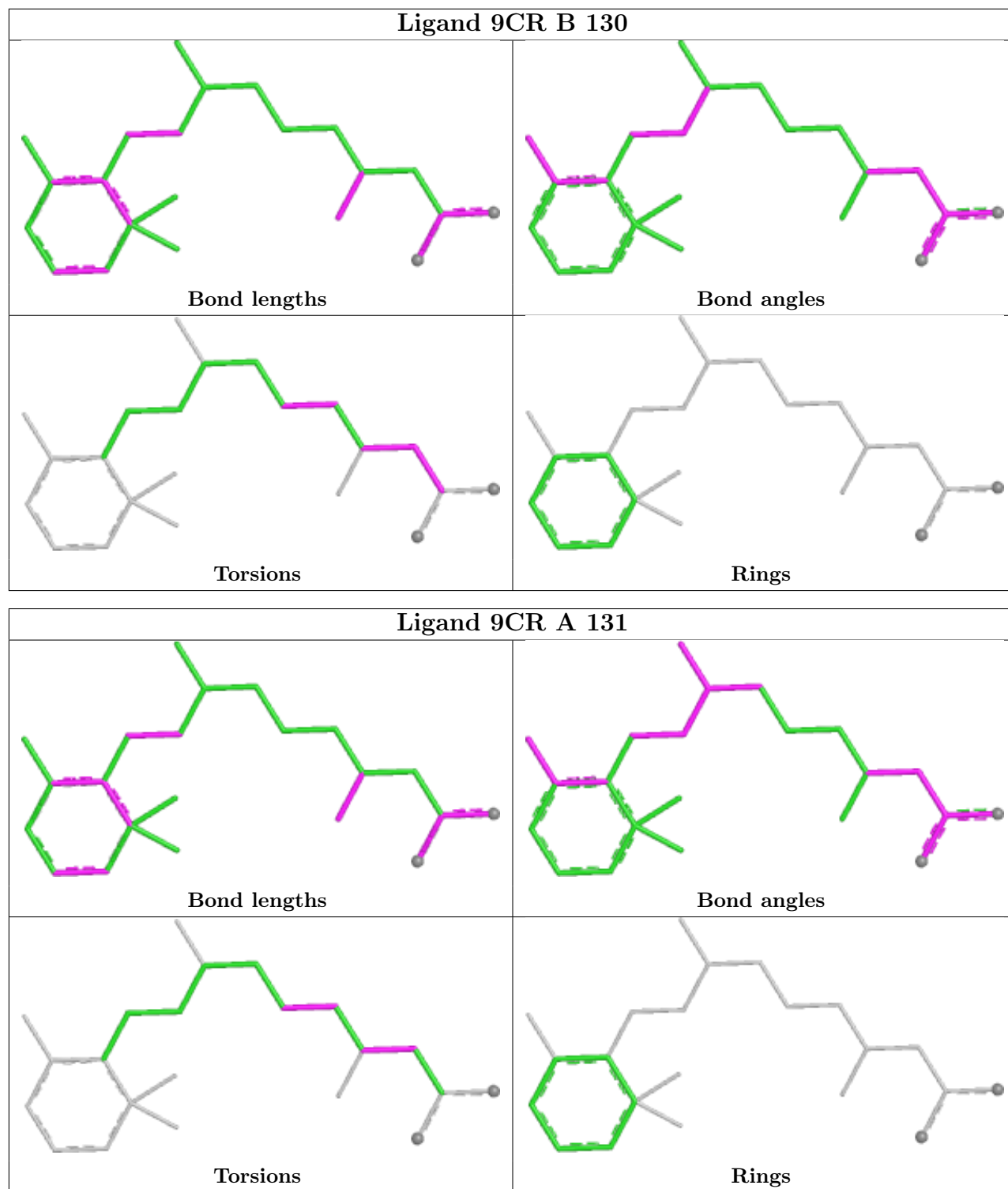
Mol	Chain	Res	Type	Atoms
2	B	130	9CR	C12-C13-C14-C15
2	B	130	9CR	C20-C13-C14-C15
2	B	130	9CR	C13-C14-C15-O1
2	B	130	9CR	C13-C14-C15-O2
2	A	131	9CR	C10-C11-C12-C13
2	B	130	9CR	C10-C11-C12-C13

There are no ring outliers.

2 monomers are involved in 83 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	130	9CR	17	26
2	A	131	9CR	17	23

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 ⓘ

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.