Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:37 am BST

PDB ID	:	1TYR
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 following versions of software and data (see references ⓘ) were used in the production of this report:

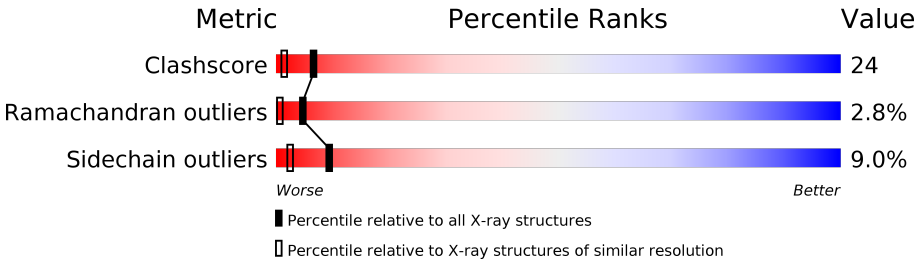
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 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	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (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 on 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	127	56% 31% 9%
1	B	127	51% 39% 8%

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

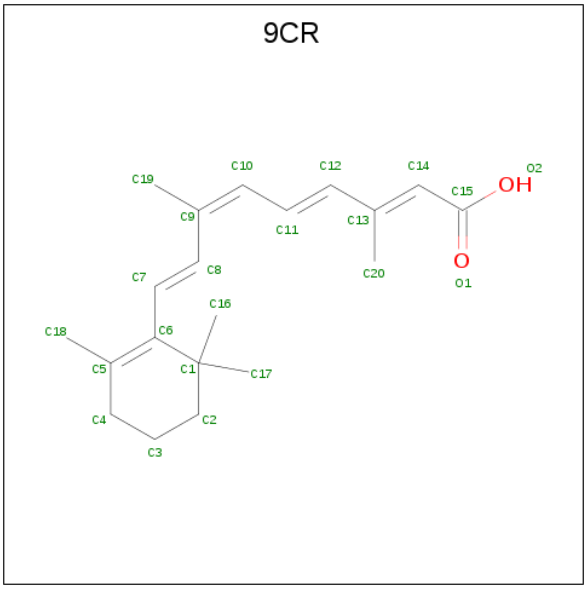
There are 3 unique types of molecules in this entry. The entry contains 2085 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: 9CR) (formula: $C_{20}H_{28}O_2$).



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 O 53 53	0	0
3	B	44	Total O 44 44	0	0

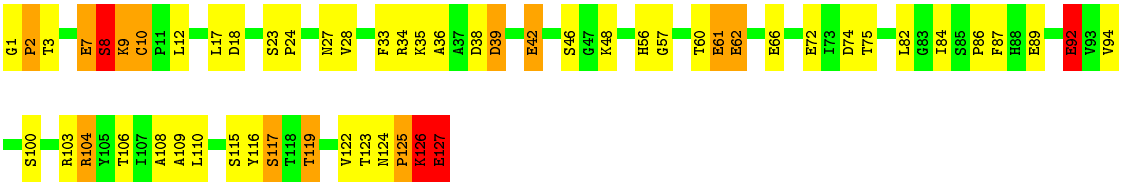
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

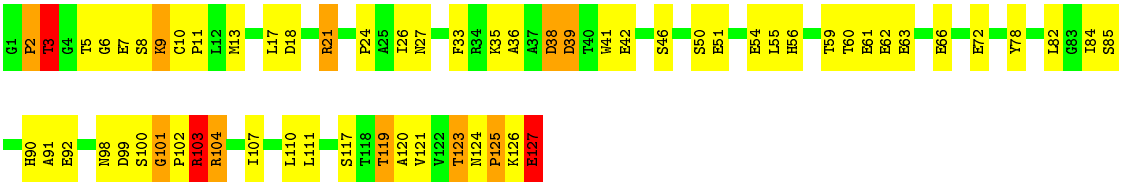
- Molecule 1: TRANSTHYRETIN

Chain A:



- Molecule 1: TRANSTHYRETIN

Chain B:



4 Data and refinement statistics (i)

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	7.23	10/997 (1.0%)	2.09	36/1357 (2.7%)
1	B	2.79	11/997 (1.1%)	1.95	30/1357 (2.2%)
All	All	5.48	21/1994 (1.1%)	2.02	66/2714 (2.4%)

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 (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	GLU	C-OXT	225.18	5.51	1.23
1	B	127	GLU	C-OXT	79.41	2.74	1.23
1	B	7	GLU	CD-OE1	8.21	1.34	1.25
1	A	42	GLU	CD-OE1	7.79	1.34	1.25
1	B	63	GLU	CD-OE1	7.70	1.34	1.25
1	B	127	GLU	CD-OE1	7.32	1.33	1.25
1	A	92	GLU	CD-OE2	7.07	1.33	1.25
1	A	62	GLU	CD-OE2	6.77	1.33	1.25
1	B	42	GLU	CD-OE1	6.75	1.33	1.25
1	B	51	GLU	CD-OE2	6.73	1.33	1.25
1	A	7	GLU	CD-OE2	6.66	1.32	1.25
1	A	89	GLU	CD-OE1	-6.61	1.18	1.25
1	A	66	GLU	CD-OE2	6.61	1.32	1.25
1	B	62	GLU	CD-OE2	6.56	1.32	1.25
1	A	61	GLU	CD-OE2	6.54	1.32	1.25
1	A	127	GLU	CD-OE1	6.09	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	72	GLU	CD-OE2	5.99	1.32	1.25
1	A	72	GLU	CD-OE2	5.89	1.32	1.25
1	B	85	SER	CB-OG	-5.87	1.34	1.42
1	B	61	GLU	CD-OE2	5.72	1.31	1.25
1	B	66	GLU	CD-OE2	5.43	1.31	1.25

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	34	ARG	NE-CZ-NH2	-13.67	113.47	120.30
1	A	103	ARG	NE-CZ-NH1	11.67	126.14	120.30
1	A	116	TYR	CB-CG-CD2	-11.67	114.00	121.00
1	A	103	ARG	NE-CZ-NH2	-10.63	114.98	120.30
1	A	34	ARG	NE-CZ-NH1	10.62	125.61	120.30
1	B	103	ARG	NE-CZ-NH1	9.96	125.28	120.30
1	A	39	ASP	CB-CG-OD2	-9.56	109.69	118.30
1	B	21	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	A	119	THR	OG1-CB-CG2	-8.10	91.38	110.00
1	B	10	CYS	CA-CB-SG	-7.88	99.81	114.00
1	A	33	PHE	CB-CG-CD2	-7.86	115.30	120.80
1	B	38	ASP	CB-CG-OD2	-7.80	111.28	118.30
1	B	42	GLU	N-CA-CB	-7.78	96.60	110.60
1	A	60	THR	CA-CB-CG2	-7.73	101.58	112.40
1	A	117	SER	N-CA-CB	-7.23	99.66	110.50
1	B	99	ASP	CB-CG-OD1	7.08	124.67	118.30
1	B	24	PRO	N-CA-CB	6.95	111.64	103.30
1	A	10	CYS	CA-CB-SG	-6.90	101.58	114.00
1	A	116	TYR	N-CA-CB	6.75	122.75	110.60
1	B	39	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	B	119	THR	CA-CB-OG1	-6.63	95.07	109.00
1	B	46	SER	N-CA-CB	6.63	120.44	110.50
1	B	98	ASN	CB-CA-C	-6.36	97.69	110.40
1	B	3	THR	CA-CB-OG1	6.34	122.31	109.00
1	B	117	SER	N-CA-CB	-6.29	101.06	110.50
1	B	39	ASP	CB-CG-OD1	6.27	123.94	118.30
1	A	46	SER	N-CA-CB	6.24	119.85	110.50
1	A	38	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	A	86	PRO	N-CA-CB	-6.17	95.81	102.60
1	B	18	ASP	CB-CG-OD2	-6.16	112.75	118.30
1	A	18	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	B	38	ASP	CB-CG-OD1	6.03	123.73	118.30
1	A	34	ARG	CG-CD-NE	-6.03	99.14	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	78	TYR	CB-CG-CD2	6.02	124.61	121.00
1	A	8	SER	CB-CA-C	-5.85	98.99	110.10
1	A	33	PHE	CB-CG-CD1	5.84	124.89	120.80
1	A	75	THR	CA-CB-CG2	-5.75	104.35	112.40
1	A	39	ASP	CB-CG-OD1	5.74	123.47	118.30
1	A	116	TYR	CB-CG-CD1	5.74	124.44	121.00
1	A	82	LEU	CB-CA-C	-5.67	99.42	110.20
1	B	102	PRO	N-CA-CB	5.67	110.11	103.30
1	B	18	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	18	ASP	CB-CG-OD1	5.61	123.35	118.30
1	B	6	GLY	C-N-CA	5.58	135.66	121.70
1	A	123	THR	N-CA-CB	-5.56	99.73	110.30
1	A	106	THR	CA-CB-CG2	-5.54	104.65	112.40
1	A	28	VAL	CA-CB-CG2	-5.52	102.61	110.90
1	B	72	GLU	CB-CG-CD	-5.52	99.30	114.20
1	B	33	PHE	CB-CG-CD2	-5.51	116.94	120.80
1	A	62	GLU	CG-CD-OE1	5.48	129.26	118.30
1	B	78	TYR	CG-CD2-CE2	5.47	125.68	121.30
1	A	122	VAL	CG1-CB-CG2	-5.47	102.15	110.90
1	A	56	HIS	CB-CA-C	-5.44	99.53	110.40
1	B	111	LEU	CB-CA-C	-5.42	99.90	110.20
1	A	94	VAL	CG1-CB-CG2	-5.41	102.24	110.90
1	B	7	GLU	CB-CA-C	5.38	121.16	110.40
1	B	107	ILE	CB-CA-C	-5.29	101.02	111.60
1	A	38	ASP	CB-CG-OD1	5.28	123.06	118.30
1	B	127	GLU	N-CA-CB	5.27	120.08	110.60
1	B	123	THR	CA-CB-CG2	-5.24	105.06	112.40
1	A	87	PHE	CB-CG-CD1	-5.23	117.14	120.80
1	A	74	ASP	CB-CG-OD1	5.19	122.97	118.30
1	B	62	GLU	CA-CB-CG	-5.09	102.20	113.40
1	B	91	ALA	N-CA-CB	5.09	117.23	110.10
1	A	104	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	12	LEU	CB-CG-CD1	-5.03	102.46	111.00

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 (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	972	0	945	32	0
1	B	972	0	945	55	0
2	A	22	0	28	17	23
2	B	22	0	28	16	26
3	A	53	0	0	3	0
3	B	44	0	0	3	5
All	All	2085	0	1946	92	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 (92) 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:H26	2:A:131:9CR:H9	1.31	1.08
1:A:17:LEU:HD11	2:A:131:9CR:H26	1.39	1.02
2:B:130:9CR:C20	2:B:130:9CR:H9	1.89	1.02
2:A:131:9CR:C20	2:A:131:9CR:H9	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:121:VAL:HG21	2:B:130:9CR:H25	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG3	1:B:103:ARG:HH11	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:N	1:A:92:GLU:OE1	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:C10	2:A:131:9CR:C20	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
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:CG	1:B:103:ARG:HH11	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:13:MET:HB2	1:B:104:ARG:CZ	2.35	0.54
1:B:11:PRO:HG2	1:B:59:THR:HG23	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:108:ALA:HB3	2:A:131:9CR:C16	2.33	0.48
1:A:2:PRO:O	1:A:62:GLU:HG2	2.13	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:HE2	1:A:9:LYS:HB2	1.82	0.45
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:A:109:ALA:C	2:A:131:9CR:H17	2.38	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
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:124:ASN:N	1:B:125:PRO:CD	2.80	0.41
1:B:26:ILE:O	1:B:27:ASN:HB2	2.19	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:B:130:9CR:C17	2:B:130:9CR:C18[2_665]	0.39	1.81
2:A:131:9CR:C9	2:A:131:9CR:C9[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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:130:9CR:C5	2:B:130:9CR:C17[2_665]	1.82	0.38
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:130:9CR:C9	2:B:130:9CR:C19[2_665]	2.18	0.02
2:A:131:9CR:C19	2:A:131:9CR:C20[2_665]	2.18	0.02

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	125/127 (98%)	118 (94%)	4 (3%)	3 (2%)	6 1
1	B	125/127 (98%)	109 (87%)	12 (10%)	4 (3%)	4 0
All	All	250/254 (98%)	227 (91%)	16 (6%)	7 (3%)	5 1

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

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%)	94 (90%)	11 (10%)	7 1
1	B	105/105 (100%)	97 (92%)	8 (8%)	13 4
All	All	210/210 (100%)	191 (91%)	19 (9%)	9 2

All (19) 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	35	LYS
1	A	39	ASP
1	A	61	GLU
1	A	92	GLU
1	A	100	SER
1	A	104	ARG
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	104	ARG
1	B	126	LYS
1	B	127	GLU

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

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

5.3.3 RNA

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 carbohydrates 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	131	-	19,22,22	2.33	5 (26%)	26,30,30	1.20	3 (11%)
2	9CR	B	130	1	19,22,22	2.34	5 (26%)	26,30,30	1.20	3 (11%)

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	131	-	-	3/13/32/32	0/1/1/1
2	9CR	B	130	1	-	3/13/32/32	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	130	9CR	C1-C6	5.58	1.61	1.53
2	A	131	9CR	C1-C6	5.56	1.61	1.53
2	B	130	9CR	C8-C7	5.32	1.49	1.33
2	A	131	9CR	C8-C7	5.31	1.49	1.33
2	A	131	9CR	C20-C13	3.49	1.58	1.50
2	B	130	9CR	C2-C3	-3.48	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	131	9CR	C2-C3	-3.48	1.44	1.52
2	B	130	9CR	C20-C13	3.43	1.58	1.50
2	B	130	9CR	C5-C6	2.98	1.39	1.34
2	A	131	9CR	C5-C6	2.98	1.39	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	131	9CR	C7-C8-C9	3.69	131.81	126.23
2	B	130	9CR	C7-C8-C9	3.68	131.80	126.23
2	A	131	9CR	C19-C9-C10	2.25	126.07	122.92
2	B	130	9CR	C19-C9-C10	2.20	126.01	122.92
2	A	131	9CR	C18-C5-C6	2.13	126.92	124.53
2	B	130	9CR	C18-C5-C6	2.10	126.89	124.53

There are no chirality outliers.

All (6) 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
2	B	130	9CR	C12-C13-C14-C15
2	B	130	9CR	C20-C13-C14-C15
2	A	131	9CR	C10-C11-C12-C13
2	B	130	9CR	C10-C11-C12-C13

There are no ring outliers.

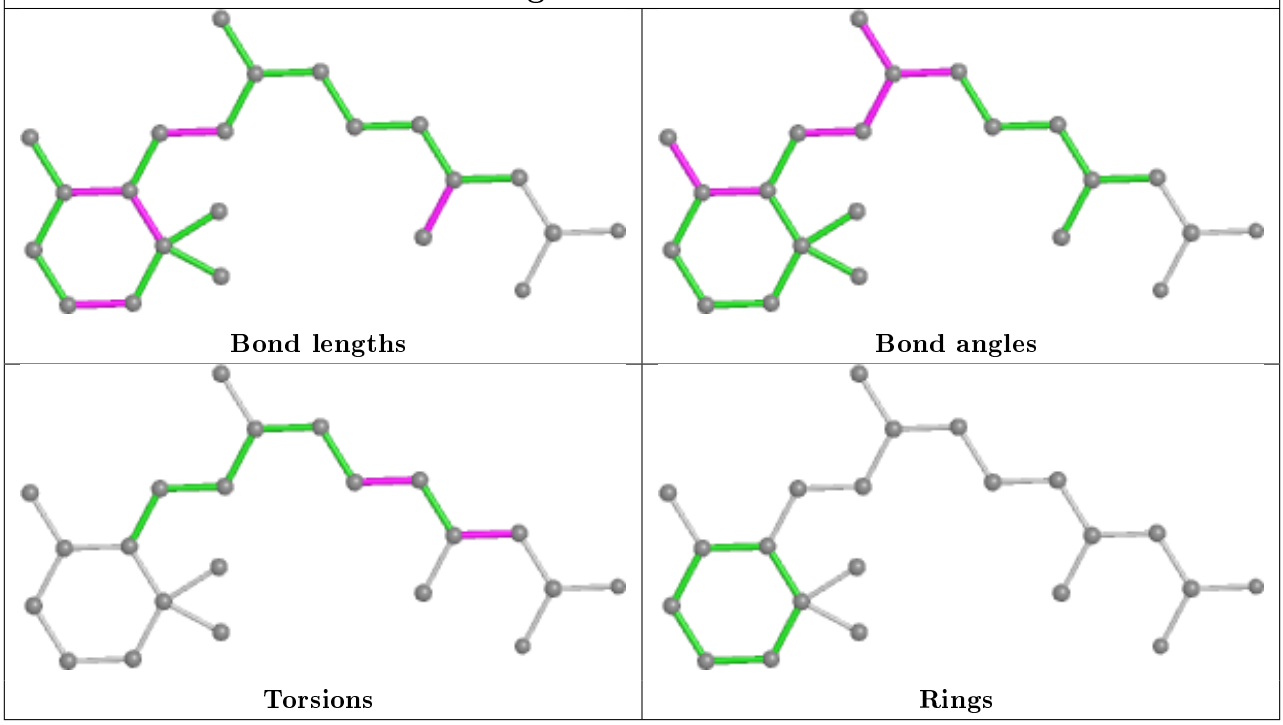
2 monomers are involved in 82 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	131	9CR	17	23
2	B	130	9CR	16	26

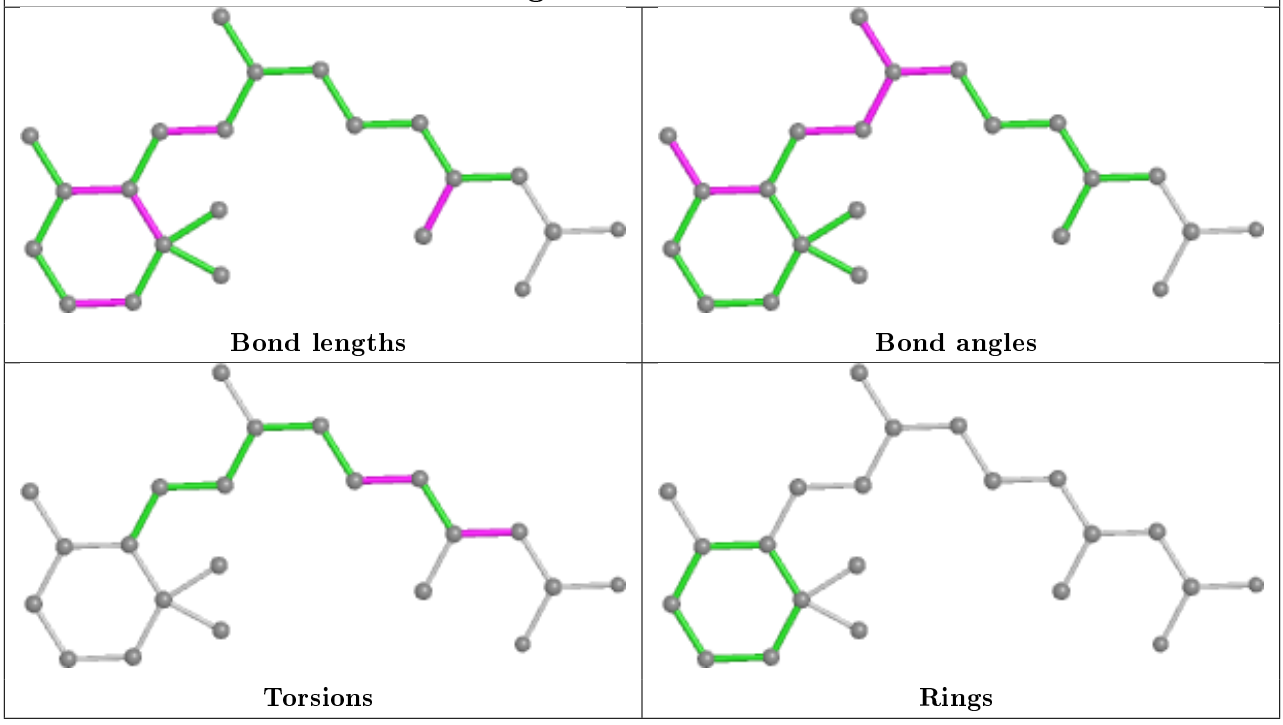
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 9CR A 131



Ligand 9CR B 130



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.