



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 05:41 pm BST

PDB ID : 2ROY
Title : TRANSTHYRETIN (ALSO CALLED PREALBUMIN) COMPLEX WITH 3
'5'-DINITRO-N-ACETYL-L-THYRONINE
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Deposited on : 1996-10-23
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 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)
Xtrriage (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

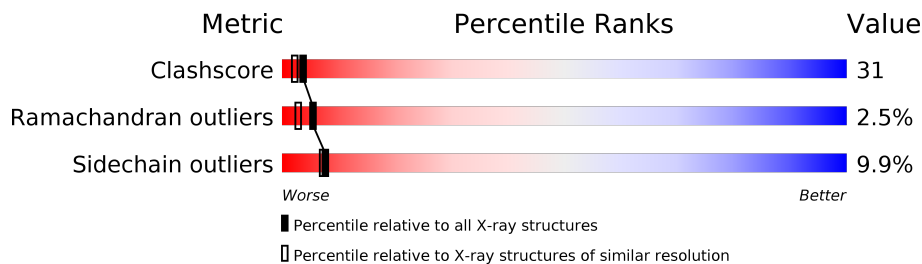
1 Overall quality at a glance

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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (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 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	127	
1	B	127	

2 Entry composition [i](#)

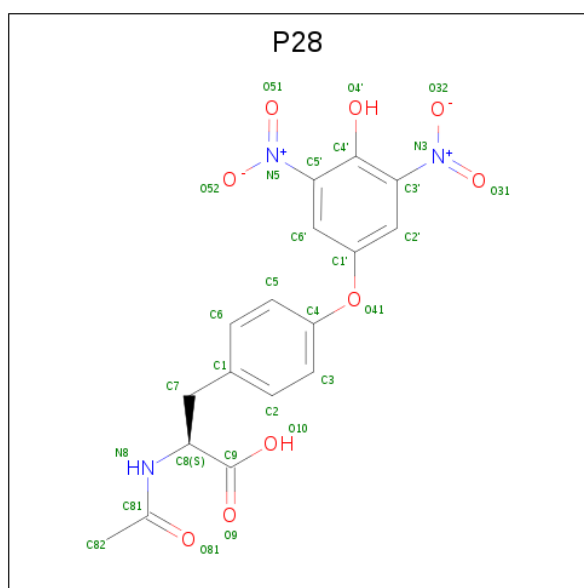
There are 3 unique types of molecules in this entry. The entry contains 1998 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	121	Total 938	C 598	N 154	O 184	S 2	0	0	0
1	B	119	Total 920	C 587	N 151	O 180	S 2	0	0	0

- Molecule 2 is 3',5'-DINITRO-N-ACETYL-L-THYRONINE (three-letter code: P28) (formula: C₁₇H₁₅N₃O₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 29	C 17	N 3	O 9	0	0
2	B	1	Total 29	C 17	N 3	O 9	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	44	Total 44	O 44	0	0
3	B	38	Total 38	O 38	0	0

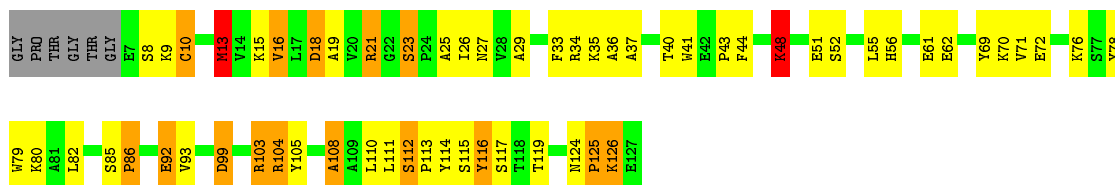
3 Residue-property plots [i](#)

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.

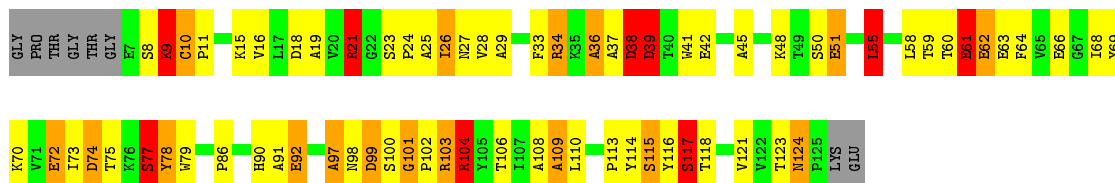
- Molecule 1: TRANSTHYRETIN

Chain A: 



- Molecule 1: TRANSTHYRETIN

Chain B: 



4 Data and refinement statistics

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	43.62Å 86.04Å 64.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.184 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1998	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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: P28

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	1.02	0/962	2.28	46/1310 (3.5%)
1	B	1.04	0/944	2.31	46/1287 (3.6%)
All	All	1.03	0/1906	2.30	92/2597 (3.5%)

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	2

There are no bond length outliers.

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	62	GLU	CB-CG-CD	15.21	155.26	114.20
1	A	99	ASP	CB-CG-OD2	-11.12	108.29	118.30
1	B	51	GLU	OE1-CD-OE2	10.87	136.34	123.30
1	A	21	ARG	NE-CZ-NH1	10.62	125.61	120.30
1	B	99	ASP	N-CA-CB	9.29	127.33	110.60
1	A	18	ASP	CB-CG-OD2	-8.96	110.24	118.30
1	B	103	ARG	NE-CZ-NH2	-8.75	115.92	120.30
1	A	21	ARG	CD-NE-CZ	8.72	135.81	123.60
1	B	39	ASP	CB-CG-OD1	8.63	126.06	118.30
1	B	77	SER	N-CA-CB	8.49	123.23	110.50
1	A	105	TYR	CB-CG-CD2	8.04	125.82	121.00
1	B	38	ASP	CB-CG-OD2	-8.02	111.08	118.30
1	A	78	TYR	CB-CG-CD2	8.00	125.80	121.00
1	A	78	TYR	CB-CG-CD1	-7.99	116.20	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	42	GLU	CA-CB-CG	7.98	130.95	113.40
1	B	106	THR	O-C-N	7.79	135.16	122.70
1	A	116	TYR	CB-CG-CD2	-7.63	116.42	121.00
1	A	104	ARG	CD-NE-CZ	-7.51	113.08	123.60
1	B	9	LYS	N-CA-CB	7.40	123.92	110.60
1	B	92	GLU	OE1-CD-OE2	7.35	132.12	123.30
1	B	109	ALA	CB-CA-C	7.27	121.01	110.10
1	A	103	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	B	62	GLU	CG-CD-OE1	6.97	132.25	118.30
1	B	99	ASP	CA-C-N	-6.94	101.92	117.20
1	B	97	ALA	CB-CA-C	6.91	120.46	110.10
1	A	61	GLU	CG-CD-OE2	-6.87	104.57	118.30
1	B	72	GLU	CG-CD-OE2	-6.81	104.67	118.30
1	A	93	VAL	CA-CB-CG1	6.75	121.02	110.90
1	B	61	GLU	CA-CB-CG	6.69	128.12	113.40
1	A	10	CYS	O-C-N	6.63	133.69	121.10
1	A	13	MET	CB-CA-C	6.53	123.45	110.40
1	A	61	GLU	OE1-CD-OE2	6.45	131.04	123.30
1	A	44	PHE	CB-CG-CD1	-6.43	116.30	120.80
1	B	72	GLU	OE1-CD-OE2	6.36	130.93	123.30
1	B	21	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	44	PHE	CB-CA-C	6.16	122.73	110.40
1	A	86	PRO	N-CA-CB	-6.11	95.88	102.60
1	A	37	ALA	CB-CA-C	6.09	119.23	110.10
1	B	91	ALA	N-CA-CB	6.09	118.62	110.10
1	B	16	VAL	CG1-CB-CG2	-6.01	101.29	110.90
1	A	27	ASN	CB-CA-C	5.98	122.35	110.40
1	B	103	ARG	NH1-CZ-NH2	5.97	125.97	119.40
1	A	112	SER	N-CA-CB	5.92	119.39	110.50
1	A	85	SER	N-CA-C	-5.92	95.02	111.00
1	A	71	VAL	N-CA-C	-5.89	95.09	111.00
1	B	106	THR	CA-C-N	-5.82	104.39	117.20
1	A	48	LYS	CA-CB-CG	5.81	126.19	113.40
1	B	21	ARG	CD-NE-CZ	5.80	131.72	123.60
1	A	56	HIS	CB-CA-C	-5.80	98.81	110.40
1	B	104	ARG	CD-NE-CZ	-5.79	115.49	123.60
1	A	108	ALA	CB-CA-C	-5.79	101.41	110.10
1	A	18	ASP	CB-CG-OD1	5.79	123.51	118.30
1	B	38	ASP	C-N-CA	5.78	136.14	121.70
1	B	62	GLU	OE1-CD-OE2	-5.74	116.41	123.30
1	B	36	ALA	CB-CA-C	5.73	118.69	110.10
1	A	44	PHE	O-C-N	-5.71	113.56	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	VAL	CG1-CB-CG2	-5.67	101.83	110.90
1	A	34	ARG	NE-CZ-NH1	-5.63	117.48	120.30
1	A	103	ARG	NH1-CZ-NH2	5.63	125.59	119.40
1	B	77	SER	CB-CA-C	-5.63	99.41	110.10
1	B	24	PRO	N-CA-C	-5.61	97.50	112.10
1	A	61	GLU	CB-CA-C	-5.58	99.25	110.40
1	A	79	TRP	CD1-NE1-CE2	5.57	114.01	109.00
1	B	110	LEU	CA-C-O	-5.57	108.41	120.10
1	A	114	TYR	CB-CG-CD1	5.55	124.33	121.00
1	A	114	TYR	CB-CG-CD2	-5.52	117.69	121.00
1	A	23	SER	N-CA-CB	-5.48	102.29	110.50
1	B	117	SER	N-CA-CB	5.45	118.68	110.50
1	A	104	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	B	19	ALA	C-N-CA	5.41	135.24	121.70
1	B	10	CYS	N-CA-CB	5.41	120.34	110.60
1	A	72	GLU	O-C-N	5.38	131.31	122.70
1	A	103	ARG	NE-CZ-NH1	-5.37	117.61	120.30
1	A	70	LYS	CA-CB-CG	-5.33	101.67	113.40
1	B	55	LEU	CA-C-O	-5.33	108.90	120.10
1	B	45	ALA	N-CA-CB	-5.33	102.64	110.10
1	B	118	THR	CA-CB-OG1	-5.31	97.84	109.00
1	B	25	ALA	N-CA-CB	5.30	117.53	110.10
1	A	115	SER	N-CA-CB	-5.29	102.57	110.50
1	A	16	VAL	CA-CB-CG1	5.28	118.83	110.90
1	B	99	ASP	C-N-CA	5.28	134.89	121.70
1	B	74	ASP	CB-CG-OD2	5.27	123.05	118.30
1	B	109	ALA	N-CA-CB	-5.27	102.73	110.10
1	B	114	TYR	CB-CG-CD2	5.24	124.14	121.00
1	B	116	TYR	CA-CB-CG	5.18	123.25	113.40
1	A	71	VAL	CA-CB-CG1	5.17	118.65	110.90
1	A	111	LEU	CB-CA-C	-5.16	100.40	110.20
1	A	62	GLU	CB-CG-CD	5.16	128.12	114.20
1	B	113	PRO	N-CD-CG	-5.15	95.48	103.20
1	B	78	TYR	CB-CA-C	5.05	120.51	110.40
1	A	13	MET	CB-CG-SD	-5.05	97.25	112.40
1	B	34	ARG	NE-CZ-NH2	5.01	122.81	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	104	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	21	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	938	0	912	38	0
1	B	920	0	893	81	0
2	A	29	0	13	8	0
2	B	29	0	13	6	0
3	A	44	0	0	1	0
3	B	38	0	0	8	0
All	All	1998	0	1831	117	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 31.

All (117) 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:B:9:LYS:HE3	1:B:104:ARG:HH11	1.08	1.13
1:B:103:ARG:HG3	1:B:124:ASN:HA	1.29	1.13
1:B:21:ARG:NH2	1:B:78:TYR:OH	2.01	0.92
1:B:9:LYS:HD3	1:B:61:GLU:HG2	1.50	0.91
1:B:9:LYS:HE3	1:B:104:ARG:HD3	1.52	0.89
1:B:9:LYS:HG2	1:B:11:PRO:HD3	1.57	0.86
1:A:124:ASN:OD1	1:A:125:PRO:HD2	1.74	0.85
1:B:10:CYS:SG	3:B:165:HOH:O	2.36	0.83
1:B:103:ARG:CG	1:B:124:ASN:HA	2.11	0.80
1:B:9:LYS:CE	1:B:104:ARG:HH11	1.92	0.78
1:B:9:LYS:HE3	1:B:104:ARG:NH1	1.94	0.78
1:B:10:CYS:O	1:B:104:ARG:HD2	1.86	0.76
1:B:10:CYS:HB2	3:B:165:HOH:O	1.86	0.76
1:B:37:ALA:C	1:B:39:ASP:H	1.86	0.76
1:B:18:ASP:OD2	1:B:21:ARG:NH2	2.14	0.74
1:A:108:ALA:CB	2:A:128:P28:H3	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ALA:HB1	2:A:128:P28:H3	1.71	0.73
1:B:37:ALA:O	1:B:39:ASP:N	2.25	0.70
1:A:33:PHE:O	1:A:69:TYR:HA	1.91	0.69
1:B:108:ALA:HB2	2:B:128:P28:H2	1.75	0.69
1:B:34:ARG:HG2	1:B:34:ARG:NH1	2.07	0.68
1:B:59:THR:CG2	1:B:60:THR:H	2.05	0.68
1:B:103:ARG:HG3	1:B:124:ASN:CA	2.17	0.67
1:A:103:ARG:HA	1:A:125:PRO:HD3	1.75	0.67
1:A:26:ILE:HD11	1:A:51:GLU:O	1.95	0.66
1:B:37:ALA:C	1:B:39:ASP:N	2.48	0.65
1:B:34:ARG:HG2	1:B:34:ARG:HH11	1.61	0.64
1:B:36:ALA:O	1:B:39:ASP:HA	1.97	0.64
1:B:74:ASP:OD2	1:B:77:SER:OG	2.15	0.64
1:B:59:THR:CG2	1:B:60:THR:N	2.60	0.64
1:B:9:LYS:CE	1:B:104:ARG:HD3	2.27	0.63
1:B:27:ASN:ND2	3:B:130:HOH:O	2.31	0.63
1:B:103:ARG:HB2	1:B:123:THR:O	1.98	0.62
1:B:8:SER:O	1:B:9:LYS:C	2.37	0.62
1:B:90:HIS:NE2	1:B:92:GLU:CD	2.52	0.62
1:A:26:ILE:HD13	1:A:51:GLU:HA	1.83	0.61
1:B:66:GLU:HA	1:B:97:ALA:O	2.01	0.61
1:A:76:LYS:O	1:A:80:LYS:HG2	2.01	0.60
1:B:28:VAL:O	1:B:48:LYS:HA	2.01	0.60
1:B:72:GLU:OE2	3:B:158:HOH:O	2.16	0.60
1:B:10:CYS:O	1:B:104:ARG:CD	2.51	0.59
1:B:59:THR:HG22	1:B:60:THR:N	2.18	0.57
1:A:117:SER:HB3	1:B:117:SER:HB3	1.86	0.57
1:B:29:ALA:HB2	1:B:48:LYS:HE3	1.86	0.57
1:B:70:LYS:HE2	1:B:92:GLU:OE2	2.05	0.57
1:B:108:ALA:HB1	2:B:128:P28:H3	1.86	0.57
1:B:18:ASP:OD2	1:B:78:TYR:OH	2.23	0.56
1:B:63:GLU:OE1	1:B:63:GLU:HA	2.06	0.56
1:B:9:LYS:HG3	1:B:10:CYS:N	2.22	0.55
1:A:15:LYS:NZ	1:A:52:SER:O	2.38	0.55
1:A:15:LYS:O	1:A:108:ALA:HA	2.06	0.54
1:A:92:GLU:OE2	1:B:92:GLU:OE1	2.25	0.53
1:B:28:VAL:HG11	1:B:73:ILE:HG23	1.90	0.53
1:B:21:ARG:HH21	1:B:78:TYR:HH	1.56	0.52
1:A:108:ALA:HB2	2:A:128:P28:H2	1.89	0.52
1:A:103:ARG:HA	1:A:125:PRO:CD	2.40	0.51
1:A:103:ARG:NH1	1:A:124:ASN:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:TYR:OH	3:A:167:HOH:O	2.11	0.51
1:B:59:THR:HG23	1:B:60:THR:H	1.73	0.51
1:A:124:ASN:OD1	1:A:125:PRO:CD	2.53	0.51
1:B:10:CYS:CB	3:B:165:HOH:O	2.45	0.51
1:A:36:ALA:N	1:A:40:THR:O	2.24	0.50
1:B:59:THR:HG22	1:B:60:THR:O	2.11	0.50
1:A:108:ALA:HB2	2:A:128:P28:C2	2.42	0.50
1:B:9:LYS:HG2	1:B:11:PRO:CD	2.37	0.49
1:B:62:GLU:OE2	3:B:140:HOH:O	2.20	0.49
1:A:16:VAL:HG12	1:A:25:ALA:HB3	1.93	0.49
1:B:9:LYS:HE3	1:B:104:ARG:CD	2.32	0.49
1:B:59:THR:HG21	1:B:64:PHE:HB2	1.95	0.48
1:B:79:TRP:HB2	1:B:86:PRO:HG3	1.95	0.48
1:A:35:LYS:HE2	1:A:41:TRP:CZ2	2.48	0.48
1:A:19:ALA:HB2	1:A:110:LEU:HD11	1.95	0.48
1:B:74:ASP:HB2	3:B:132:HOH:O	2.13	0.47
1:B:9:LYS:CG	1:B:10:CYS:N	2.77	0.47
1:B:99:ASP:OD1	1:B:101:GLY:C	2.52	0.47
1:B:109:ALA:HA	1:B:117:SER:O	2.14	0.47
1:B:9:LYS:HE2	1:B:11:PRO:HB3	1.97	0.47
1:B:26:ILE:HG23	1:B:26:ILE:HD13	1.63	0.46
1:A:99:ASP:OD1	1:A:99:ASP:N	2.48	0.46
1:B:41:TRP:CH2	1:B:68:ILE:HG22	2.51	0.46
1:A:108:ALA:CB	2:A:128:P28:C3	2.93	0.45
1:B:55:LEU:HD13	1:B:58:LEU:HD21	1.99	0.45
1:A:21:ARG:HH11	1:A:82:LEU:CD2	2.30	0.44
1:B:108:ALA:CB	2:B:128:P28:C2	2.95	0.44
2:B:128:P28:C3	2:B:128:P28:H2'	2.47	0.44
1:B:26:ILE:HB	1:B:50:SER:O	2.17	0.44
1:A:108:ALA:HB2	2:A:128:P28:H3	1.99	0.44
1:B:98:ASN:O	1:B:102:PRO:HD2	2.17	0.44
1:B:73:ILE:HG22	1:B:75:THR:CG2	2.48	0.44
1:A:48:LYS:O	1:A:55:LEU:HD13	2.18	0.44
1:B:8:SER:O	1:B:9:LYS:O	2.35	0.44
1:B:15:LYS:O	1:B:108:ALA:HA	2.17	0.44
1:B:11:PRO:HA	1:B:104:ARG:CD	2.48	0.44
1:B:28:VAL:CG1	1:B:73:ILE:HG23	2.48	0.44
1:A:119:THR:HA	1:B:115:SER:HB2	1.99	0.43
1:A:117:SER:HA	1:B:117:SER:HA	1.99	0.43
1:B:75:THR:O	1:B:78:TYR:HB3	2.19	0.43
1:B:108:ALA:CB	2:B:128:P28:H2	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ILE:HG22	1:B:75:THR:HG22	2.00	0.43
2:A:128:P28:O31	2:A:128:P28:O4'	2.36	0.43
1:B:59:THR:CG2	1:B:64:PHE:HB2	2.49	0.43
1:A:8:SER:HA	1:A:13:MET:HE1	2.01	0.42
1:A:108:ALA:HB2	2:A:128:P28:C3	2.49	0.42
1:B:104:ARG:NE	3:B:154:HOH:O	2.47	0.42
1:A:18:ASP:OD2	1:A:21:ARG:HD3	2.19	0.42
1:B:99:ASP:CG	1:B:102:PRO:O	2.58	0.42
1:A:125:PRO:O	1:A:126:LYS:HG3	2.19	0.42
1:A:13:MET:HB3	1:A:13:MET:HE3	1.88	0.42
1:A:76:LYS:O	1:A:80:LYS:CG	2.67	0.42
1:A:29:ALA:HB2	1:A:48:LYS:HE3	2.01	0.41
1:A:104:ARG:HD3	1:A:104:ARG:HH11	1.45	0.41
1:B:121:VAL:HG12	1:B:123:THR:HG23	2.02	0.41
1:A:112:SER:HB3	1:A:113:PRO:HD2	2.02	0.41
1:B:108:ALA:HB2	2:B:128:P28:C2	2.48	0.41
1:B:58:LEU:HD23	1:B:58:LEU:HA	1.89	0.41
1:B:103:ARG:HG3	1:B:124:ASN:CG	2.41	0.40
1:B:33:PHE:O	1:B:69:TYR:HA	2.21	0.40

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	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	119/127 (94%)	108 (91%)	8 (7%)	3 (2%)	5	3
1	B	117/127 (92%)	105 (90%)	9 (8%)	3 (3%)	5	3
All	All	236/254 (93%)	213 (90%)	17 (7%)	6 (2%)	5	3

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	126	LYS
1	B	38	ASP
1	B	9	LYS
1	A	125	PRO
1	B	101	GLY

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	102/105 (97%)	95 (93%)	7 (7%)	15	16
1	B	100/105 (95%)	87 (87%)	13 (13%)	4	3
All	All	202/210 (96%)	182 (90%)	20 (10%)	8	7

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	CYS
1	A	13	MET
1	A	23	SER
1	A	43	PRO
1	A	48	LYS
1	A	86	PRO
1	A	92	GLU
1	B	23	SER
1	B	26	ILE
1	B	38	ASP
1	B	39	ASP
1	B	51	GLU
1	B	55	LEU
1	B	61	GLU
1	B	77	SER
1	B	100	SER
1	B	104	ARG
1	B	115	SER

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Mol	Chain	Res	Type
1	B	117	SER
1	B	124	ASN

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

Mol	Chain	Res	Type
1	A	56	HIS
1	B	27	ASN
1	B	124	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 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	P28	B	128	-	25,30,30	2.96	6 (24%)	29,42,42	3.90	9 (31%)
2	P28	A	128	-	25,30,30	2.94	6 (24%)	29,42,42	3.48	9 (31%)

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	P28	B	128	-	-	1/16/24/24	0/2/2/2
2	P28	A	128	-	-	0/16/24/24	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	128	P28	C5'-N5	-9.19	1.28	1.45
2	B	128	P28	C3'-N3	-8.71	1.29	1.45
2	B	128	P28	C5'-N5	-8.60	1.30	1.45
2	A	128	P28	C3'-N3	-8.57	1.30	1.45
2	A	128	P28	O81-C81	4.81	1.34	1.23
2	B	128	P28	O81-C81	4.53	1.33	1.23
2	B	128	P28	C7-C8	-3.93	1.48	1.53
2	B	128	P28	C8-N8	3.32	1.51	1.46
2	A	128	P28	C2'-C1'	-3.04	1.33	1.38
2	B	128	P28	C2'-C1'	-2.54	1.34	1.38
2	A	128	P28	C8-N8	2.36	1.49	1.46
2	A	128	P28	O51-N5	-2.14	1.19	1.22

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	128	P28	C8-N8-C81	-15.46	105.44	122.44
2	A	128	P28	C8-N8-C81	-14.01	107.03	122.44
2	B	128	P28	C1-C7-C8	7.32	125.42	112.97
2	B	128	P28	C7-C8-N8	7.00	121.72	109.01
2	A	128	P28	C1-C7-C8	6.47	123.97	112.97
2	B	128	P28	C7-C1-C6	-5.87	109.25	120.91
2	A	128	P28	C7-C8-N8	5.41	118.84	109.01
2	A	128	P28	C7-C1-C6	-4.86	111.25	120.91
2	B	128	P28	C7-C1-C2	4.67	130.17	120.91
2	A	128	P28	C7-C1-C2	3.27	127.39	120.91
2	A	128	P28	C3-C2-C1	-3.23	116.58	121.03
2	A	128	P28	C2-C3-C4	3.21	123.67	119.73
2	A	128	P28	C82-C81-N8	2.48	120.30	116.10
2	B	128	P28	C2-C3-C4	2.47	122.76	119.73
2	B	128	P28	O41-C4-C3	2.38	127.75	119.38
2	B	128	P28	C3-C2-C1	-2.38	117.76	121.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	128	P28	O51-N5-C5'	2.15	122.71	119.03
2	B	128	P28	O31-N3-C3'	2.08	122.58	119.03

There are no chirality outliers.

All (1) torsion outliers are listed below:

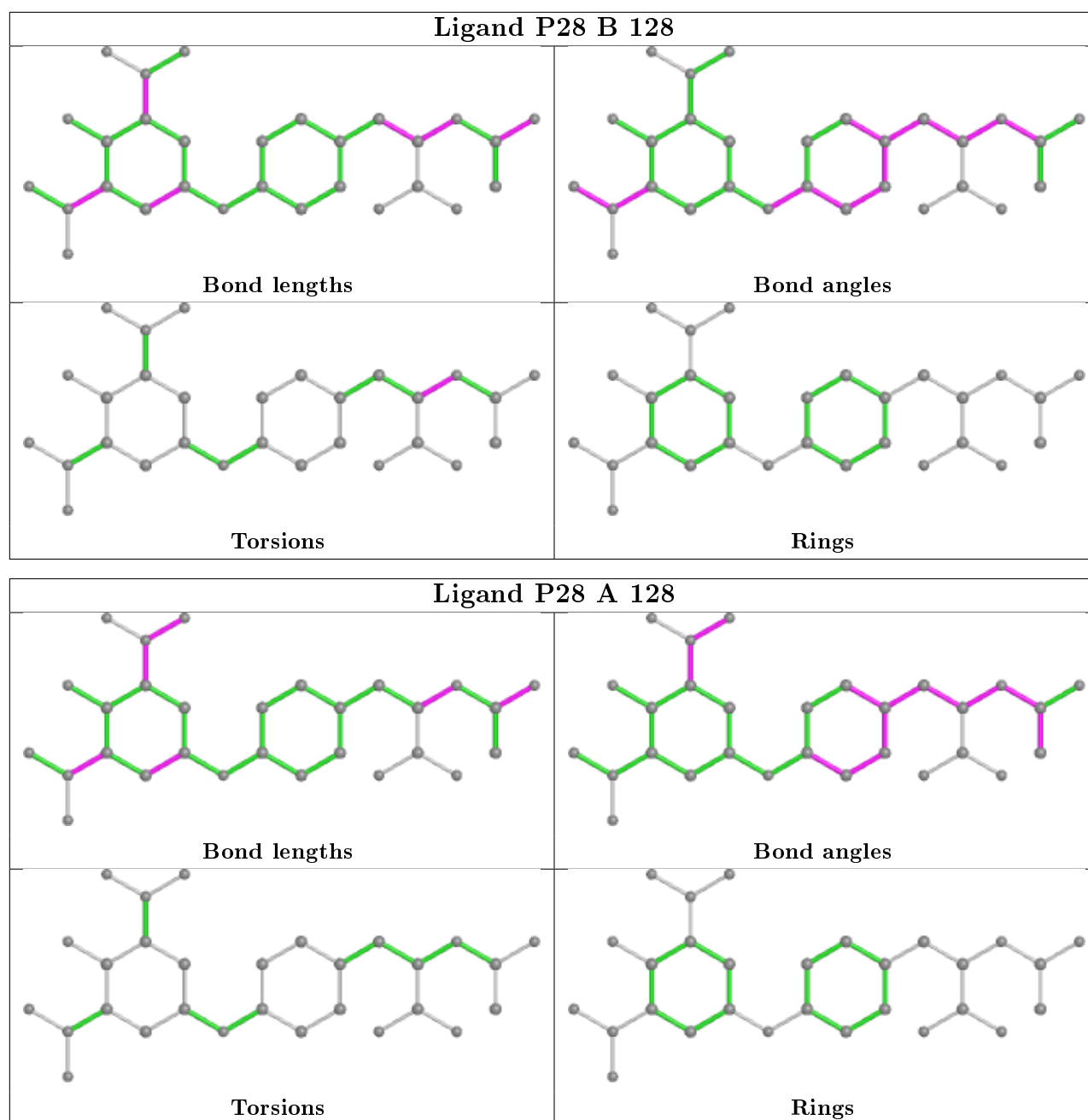
Mol	Chain	Res	Type	Atoms
2	B	128	P28	C9-C8-N8-C81

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	128	P28	6	0
2	A	128	P28	8	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 [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.