



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:42 AM UTC

PDB ID : 1THA / pdb_00001tha
Title : MECHANISM OF MOLECULAR RECOGNITION. STRUCTURAL ASPECTS OF 3,3'-DIiodo-L-THYRONINE BINDING TO HUMAN SERUM TRANSTHYRETIN
Authors : Wojtczak, A.; Luft, J.; Cody, V.
Deposited on : 1991-11-21
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

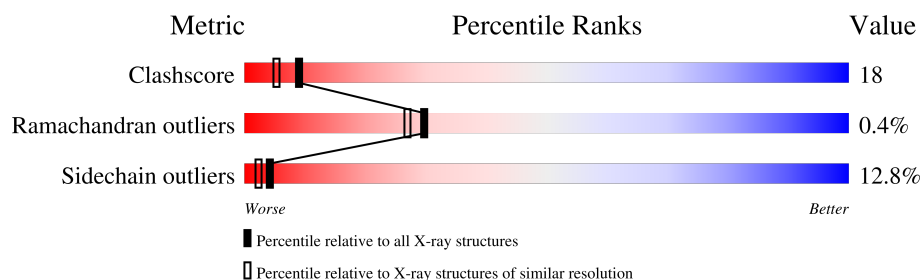
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	T33	A	130	-	X	-	-

2 Entry composition [i](#)

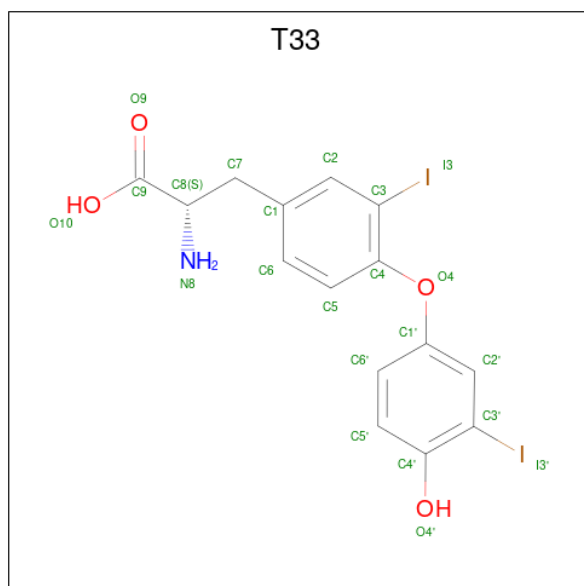
There are 3 unique types of molecules in this entry. The entry contains 1970 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	118	Total	C	N	O	S	0	3	0
			925	589	155	178	3			
1	B	116	Total	C	N	O	S	0	2	0
			903	577	148	175	3			

- Molecule 2 is 3,3'-DEIODO-THYROXINE (CCD ID: T33) (formula: $C_{15}H_{13}I_2NO_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	I	N	O	0	0
			22	15	2	1	4		
2	B	1	Total	C	I	N	O	0	0
			22	15	2	1	4		

- Molecule 3 is water.

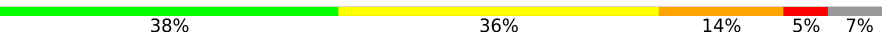
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total 50	O 50	0	0
3	B	48	Total 48	O 48	0	0

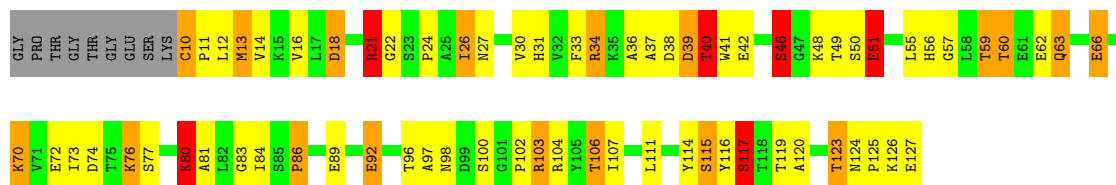
3 Residue-property plots

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.

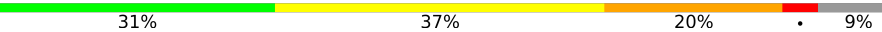
Note EDS was not executed.

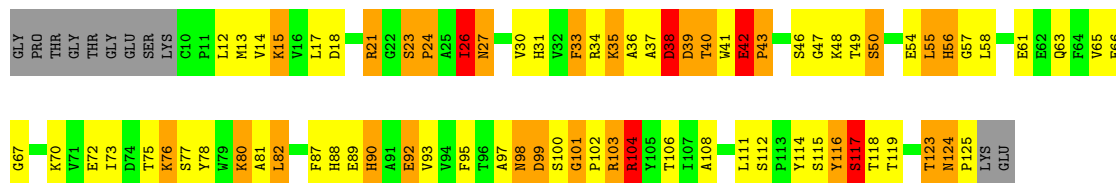
• Molecule 1: TRANSTHYRETIN

Chain A:  38% 36% 14% 5% 7%



• Molecule 1: TRANSTHYRETIN

Chain B:  31% 37% 20% • 9%



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	43.93Å 86.65Å 65.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CORELS, PROLSQ	Depositor
R, R_{free}	0.185 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1970	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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: T33

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	1.55	2/966 (0.2%)	2.80	110/1315 (8.4%)
1	B	1.46	4/937 (0.4%)	2.90	98/1278 (7.7%)
All	All	1.50	6/1903 (0.3%)	2.85	208/2593 (8.0%)

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	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	112	SER	N-CA	6.66	1.51	1.45
1	A	117	SER	C-O	5.58	1.30	1.23
1	A	18	ASP	N-CA	5.54	1.52	1.46
1	B	90	HIS	N-CA	5.53	1.52	1.46
1	B	23	SER	N-CA	5.24	1.50	1.45
1	B	75	THR	CA-CB	5.02	1.61	1.53

All (208) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	21	ARG	CD-NE-CZ	26.34	161.28	124.40
1	B	61	GLU	CA-CB-CG	12.61	139.32	114.10
1	A	50	SER	CA-C-O	10.81	135.01	121.50
1	A	12	LEU	CA-C-O	-10.50	109.11	120.24
1	B	27	ASN	OD1-CG-ND2	10.07	132.67	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	LEU	CA-C-N	10.03	139.66	122.81
1	A	55	LEU	C-N-CA	10.03	139.66	122.81
1	A	103	ARG	CD-NE-CZ	-9.93	110.50	124.40
1	A	92	GLU	CA-CB-CG	9.81	133.72	114.10
1	A	66	GLU	CA-CB-CG	9.72	133.54	114.10
1	A	41	TRP	CA-C-O	-9.52	109.84	120.60
1	B	97	ALA	CA-C-N	9.38	139.46	121.54
1	B	97	ALA	C-N-CA	9.38	139.46	121.54
1	B	41	TRP	CA-C-O	-9.35	110.30	120.30
1	A	46	SER	CA-CB-OG	-9.30	92.51	111.10
1	B	65	VAL	O-C-N	-9.29	113.48	122.12
1	A	27	ASN	OD1-CG-ND2	-9.13	113.47	122.60
1	B	42	GLU	CA-C-O	9.12	128.67	120.19
1	A	50	SER	CA-C-N	9.02	133.54	120.38
1	A	50	SER	C-N-CA	9.02	133.54	120.38
1	B	37	ALA	CA-C-N	8.99	133.23	120.28
1	B	37	ALA	C-N-CA	8.99	133.23	120.28
1	B	57	GLY	O-C-N	8.87	134.24	122.70
1	A	111	LEU	O-C-N	8.69	134.25	123.21
1	A	104	ARG	CD-NE-CZ	-8.66	112.28	124.40
1	A	49	THR	CA-C-O	8.44	130.76	121.56
1	A	39	ASP	N-CA-CB	-8.42	99.42	112.13
1	A	117	SER	CB-CA-C	8.35	126.83	109.38
1	B	104	ARG	N-CA-CB	8.34	125.38	110.95
1	A	81	ALA	CA-C-O	-8.19	110.85	120.10
1	B	76	LYS	CA-C-N	8.16	131.21	120.28
1	B	76	LYS	C-N-CA	8.16	131.21	120.28
1	A	115	SER	CA-C-O	8.16	129.96	121.23
1	B	77	SER	O-C-N	8.10	130.70	122.12
1	A	31	HIS	CA-CB-CG	-8.07	105.73	113.80
1	A	51	GLU	CB-CG-CD	8.05	126.29	112.60
1	B	104	ARG	NE-CZ-NH2	-8.05	111.96	119.20
1	B	65	VAL	CA-C-O	7.94	127.95	121.68
1	B	103	ARG	O-C-N	-7.91	112.07	122.59
1	B	72	GLU	CG-CD-OE2	-7.89	100.24	118.40
1	A	72	GLU	CB-CG-CD	-7.89	99.18	112.60
1	A	97	ALA	CA-C-N	7.89	133.68	122.08
1	A	97	ALA	C-N-CA	7.89	133.68	122.08
1	B	26	ILE	CB-CA-C	7.87	123.19	111.31
1	A	33	PHE	CA-C-O	-7.84	112.29	121.46
1	A	86	PRO	O-C-N	-7.82	113.66	123.04
1	B	115	SER	N-CA-CB	-7.77	99.49	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	PRO	CB-CA-C	-7.76	101.87	111.64
1	B	21	ARG	NE-CZ-NH2	7.73	126.16	119.20
1	B	103	ARG	N-CA-C	7.72	127.24	110.80
1	B	117	SER	CB-CA-C	7.69	125.45	109.38
1	B	104	ARG	CB-CA-C	-7.69	100.31	111.23
1	A	73	ILE	CA-C-O	-7.61	112.42	120.48
1	B	101	GLY	N-CA-C	-7.54	96.96	112.34
1	B	118	THR	O-C-N	7.46	131.92	123.27
1	B	92	GLU	CA-C-O	-7.46	112.65	120.70
1	B	46	SER	N-CA-CB	-7.36	98.51	111.39
1	B	80	LYS	CA-C-O	7.26	128.67	120.90
1	A	21	ARG	NE-CZ-NH2	7.17	125.65	119.20
1	B	90	HIS	CA-C-O	-7.14	113.64	121.28
1	B	46	SER	CA-CB-OG	7.11	125.33	111.10
1	B	111	LEU	N-CA-C	7.11	120.99	109.40
1	B	104	ARG	NE-CZ-NH1	7.10	128.60	121.50
1	B	47	GLY	CA-C-O	7.07	128.46	121.60
1	B	93	VAL	CA-C-N	7.06	133.00	122.98
1	B	93	VAL	C-N-CA	7.06	133.00	122.98
1	A	114	TYR	CA-CB-CG	-7.05	101.21	113.90
1	B	63	GLN	OE1-CD-NE2	-7.05	115.55	122.60
1	B	67	GLY	CA-C-O	-7.04	114.51	121.48
1	B	50	SER	CA-C-N	7.01	131.81	120.60
1	B	50	SER	C-N-CA	7.01	131.81	120.60
1	B	102	PRO	CB-CA-C	6.90	120.02	110.98
1	A	66	GLU	CG-CD-OE2	-6.90	102.53	118.40
1	B	103	ARG	CA-C-N	6.89	132.80	122.47
1	B	103	ARG	C-N-CA	6.89	132.80	122.47
1	B	100	SER	CA-C-N	6.88	132.68	121.87
1	B	100	SER	C-N-CA	6.88	132.68	121.87
1	A	62	GLU	CB-CG-CD	6.86	124.26	112.60
1	B	112	SER	O-C-N	-6.84	116.21	121.55
1	A	14	VAL	CA-C-O	-6.79	113.26	120.39
1	A	30	VAL	CA-C-N	6.78	132.56	123.00
1	A	30	VAL	C-N-CA	6.78	132.56	123.00
1	A	21	ARG	N-CA-C	6.77	121.70	113.38
1	A	70	LYS	CA-C-O	-6.75	113.09	120.24
1	B	119	THR	O-C-N	-6.69	115.51	123.27
1	A	83	GLY	CA-C-O	6.66	126.16	118.96
1	B	65	VAL	CA-C-N	6.59	130.19	120.90
1	B	65	VAL	C-N-CA	6.59	130.19	120.90
1	B	38	ASP	CA-CB-CG	6.49	119.09	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	26	ILE	CB-CG1-CD1	-6.46	100.22	113.80
1	B	106	THR	N-CA-CB	6.45	120.71	110.65
1	A	31	HIS	O-C-N	6.45	130.75	123.27
1	A	21	ARG	CB-CA-C	-6.44	98.45	109.65
1	B	124	ASN	N-CA-CB	6.43	121.62	110.23
1	A	39	ASP	CA-CB-CG	-6.41	106.19	112.60
1	B	116	TYR	CA-C-O	6.38	127.91	120.89
1	B	41	TRP	O-C-N	6.38	130.67	123.27
1	B	118	THR	CA-C-O	-6.38	113.66	121.06
1	A	111	LEU	N-CA-C	6.33	119.78	109.59
1	B	102	PRO	CA-C-O	-6.32	113.96	121.67
1	A	98	ASN	CA-C-O	-6.27	113.24	121.08
1	A	119	THR	O-C-N	-6.27	115.58	123.17
1	A	124	ASN	CB-CA-C	6.27	118.41	109.38
1	B	97	ALA	CB-CA-C	6.26	119.47	111.40
1	B	89	GLU	CA-C-O	6.24	127.03	120.42
1	B	24	PRO	CA-C-O	-6.23	114.17	121.95
1	B	61	GLU	CA-C-O	-6.22	113.07	120.10
1	B	125	PRO	CB-CA-C	6.22	121.92	110.10
1	A	59	THR	N-CA-C	6.17	117.25	108.74
1	A	127	GLU	CB-CG-CD	6.16	123.08	112.60
1	B	40	THR	N-CA-CB	6.06	120.03	110.39
1	A	72	GLU	CB-CA-C	-6.06	99.23	109.72
1	B	98	ASN	OD1-CG-ND2	6.06	128.66	122.60
1	B	21	ARG	NH1-CZ-NH2	-6.04	111.45	119.30
1	A	46	SER	CA-C-O	-6.00	114.27	120.99
1	A	86	PRO	CA-C-N	5.87	130.52	120.71
1	A	86	PRO	C-N-CA	5.87	130.52	120.71
1	A	77	SER	CA-C-O	-5.86	113.48	120.10
1	A	13[A]	MET	CB-CA-C	5.84	120.92	109.35
1	A	13[B]	MET	CB-CA-C	5.84	120.92	109.35
1	A	116	TYR	CA-C-N	-5.83	113.52	122.62
1	A	116	TYR	C-N-CA	-5.83	113.52	122.62
1	A	18	ASP	N-CA-CB	-5.82	101.41	110.55
1	A	18	ASP	O-C-N	-5.82	116.41	123.27
1	A	98	ASN	O-C-N	5.81	131.58	122.23
1	B	124	ASN	O-C-N	5.80	126.55	121.39
1	A	76	LYS	CA-C-N	5.79	128.62	120.28
1	A	76	LYS	C-N-CA	5.79	128.62	120.28
1	A	18	ASP	CB-CA-C	5.73	119.59	110.19
1	B	27	ASN	CA-C-O	5.72	127.91	120.81
1	A	100	SER	N-CA-C	-5.72	101.88	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	98	ASN	O-C-N	5.72	130.20	122.59
1	B	30	VAL	CB-CA-C	-5.70	102.00	110.33
1	B	15	LYS	CB-CG-CD	5.69	124.39	111.30
1	B	82	LEU	N-CA-CB	-5.67	102.10	110.49
1	A	62	GLU	CG-CD-OE1	5.67	131.44	118.40
1	B	26	ILE	CA-CB-CG2	5.65	120.10	110.50
1	A	63[A]	GLN	O-C-N	5.63	129.19	122.27
1	A	63[B]	GLN	O-C-N	5.63	129.19	122.27
1	A	12	LEU	O-C-N	5.62	129.84	123.27
1	A	16	VAL	CA-CB-CG2	5.61	119.94	110.40
1	A	27	ASN	CA-CB-CG	-5.61	106.99	112.60
1	A	62	GLU	N-CA-C	5.60	117.38	111.28
1	B	116	TYR	CB-CG-CD2	5.60	129.19	120.80
1	A	26	ILE	CA-CB-CG1	-5.57	100.93	110.40
1	B	43	PRO	CA-C-O	-5.56	115.11	121.56
1	B	100	SER	CA-CB-OG	5.56	122.21	111.10
1	B	49	THR	OG1-CB-CG2	5.53	120.35	109.30
1	B	33	PHE	CA-CB-CG	-5.52	108.28	113.80
1	B	100	SER	CA-C-O	5.49	126.63	119.98
1	B	73	ILE	CA-C-O	-5.48	114.61	120.59
1	B	65	VAL	CA-CB-CG1	5.46	119.69	110.40
1	A	111	LEU	CA-C-O	-5.46	114.92	120.71
1	A	18	ASP	CA-CB-CG	-5.45	107.15	112.60
1	A	98	ASN	CA-CB-CG	-5.45	107.15	112.60
1	B	81	ALA	O-C-N	5.44	129.47	122.39
1	A	56	HIS	CB-CA-C	-5.44	99.10	109.66
1	B	95	PHE	N-CA-C	5.42	117.30	109.07
1	A	48	LYS	CA-CB-CG	-5.41	103.28	114.10
1	A	98	ASN	CB-CG-ND2	5.41	124.51	116.40
1	A	89	GLU	N-CA-CB	5.40	118.24	110.20
1	A	102	PRO	CA-C-O	-5.40	115.45	121.23
1	A	22	GLY	O-C-N	-5.39	115.69	122.70
1	B	100	SER	N-CA-C	-5.39	102.83	111.02
1	A	50	SER	CA-CB-OG	-5.38	100.34	111.10
1	A	120	ALA	CA-C-N	5.35	130.22	123.10
1	A	120	ALA	C-N-CA	5.35	130.22	123.10
1	A	84	ILE	CA-C-O	5.33	128.24	121.48
1	A	100	SER	CA-CB-OG	5.33	121.75	111.10
1	A	123	THR	CA-CB-OG1	-5.32	101.62	109.60
1	B	106	THR	CA-CB-CG2	5.32	119.54	110.50
1	A	104	ARG	CA-CB-CG	-5.30	103.50	114.10
1	B	99	ASP	CA-C-N	5.30	128.75	122.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	99	ASP	C-N-CA	5.30	128.75	122.44
1	A	40	THR	CA-CB-CG2	5.29	119.50	110.50
1	B	88	HIS	O-C-N	5.29	129.35	122.89
1	A	76	LYS	N-CA-C	5.29	116.72	111.07
1	A	96	THR	OG1-CB-CG2	5.25	119.81	109.30
1	A	72	GLU	CG-CD-OE2	-5.24	106.34	118.40
1	B	97	ALA	N-CA-CB	-5.23	103.26	110.42
1	A	60	THR	CA-CB-OG1	-5.21	101.78	109.60
1	A	57	GLY	CA-C-N	5.20	127.20	120.44
1	A	57	GLY	C-N-CA	5.20	127.20	120.44
1	B	95	PHE	N-CA-CB	-5.20	102.98	111.66
1	A	10	CYS	CA-C-O	-5.18	111.99	120.80
1	B	76	LYS	CA-C-O	5.18	125.93	119.97
1	A	72	GLU	OE1-CD-OE2	5.16	135.29	122.90
1	A	100	SER	CA-C-O	-5.16	116.00	121.78
1	A	74	ASP	CB-CG-OD1	5.15	130.24	118.40
1	A	106	THR	CA-C-O	-5.14	114.80	120.30
1	B	76	LYS	O-C-N	-5.14	115.94	122.27
1	A	46	SER	N-CA-C	5.14	117.06	108.99
1	B	30	VAL	N-CA-C	5.13	115.51	108.12
1	B	48	LYS	CA-CB-CG	-5.12	103.85	114.10
1	A	123	THR	OG1-CB-CG2	5.12	119.54	109.30
1	A	126	LYS	N-CA-C	-5.12	102.91	110.48
1	B	43	PRO	O-C-N	5.12	129.35	123.01
1	A	18	ASP	CA-C-O	5.11	125.94	120.32
1	A	24	PRO	CB-CA-C	-5.10	104.70	111.23
1	A	102	PRO	N-CA-C	5.10	118.88	111.03
1	A	22	GLY	CA-C-O	5.07	129.39	120.57
1	A	34[A]	ARG	CB-CA-C	5.06	118.97	109.71
1	A	34[B]	ARG	CB-CA-C	5.06	118.97	109.71
1	B	46	SER	CA-C-N	5.05	130.49	120.84
1	B	46	SER	C-N-CA	5.05	130.49	120.84
1	B	88	HIS	N-CA-CB	5.04	117.38	109.97
1	A	80	LYS	CA-C-N	5.00	127.48	120.28
1	A	80	LYS	C-N-CA	5.00	127.48	120.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	34[A]	ARG	Sidechain
1	A	34[B]	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	925	0	900	22	0
1	B	903	0	878	47	0
2	A	22	0	12	0	0
2	B	22	0	11	3	0
3	A	50	0	0	3	0
3	B	48	0	0	4	0
All	All	1970	0	1801	68	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 18.

All (68) 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:103:ARG:HD3	1:B:124:ASN:HB3	1.19	1.16
1:B:103:ARG:CD	1:B:124:ASN:HB3	1.87	1.05
1:A:117:SER:HB2	1:B:117:SER:HB2	1.55	0.87
1:A:21:ARG:HG2	1:A:21:ARG:HH11	1.41	0.85
1:B:13[B]:MET:CE	1:B:54:GLU:HG2	2.06	0.84
1:B:92:GLU:HB2	3:B:154:HOH:O	1.83	0.79
1:B:116:TYR:OH	3:B:134:HOH:O	1.99	0.78
1:B:26:ILE:C	1:B:26:ILE:HD13	2.09	0.76
1:A:21:ARG:HG2	1:A:21:ARG:NH1	1.99	0.76
1:A:106:THR:HG23	3:A:137:HOH:O	1.85	0.76
1:B:13[B]:MET:HE3	1:B:56:HIS:CE1	2.23	0.73
1:A:36:ALA:HB3	1:A:40:THR:HG22	1.69	0.72
1:A:38:ASP:O	1:A:39:ASP:HB3	1.90	0.71
1:B:103:ARG:HD3	1:B:124:ASN:CB	2.11	0.71
1:B:103:ARG:O	1:B:104:ARG:HD3	1.91	0.71
1:B:38:ASP:O	1:B:39:ASP:HB2	1.92	0.69
1:B:21:ARG:NH1	1:B:78:TYR:OH	2.26	0.68
1:A:70:LYS:HD2	1:A:92:GLU:HG3	1.76	0.67
1:B:13[B]:MET:HE1	1:B:54:GLU:HG2	1.76	0.66
1:B:18:ASP:OD2	1:B:21:ARG:NH1	2.29	0.66
1:B:103:ARG:HG3	1:B:104:ARG:H	1.58	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:ALA:HB2	1:B:42:GLU:HG2	1.79	0.65
1:B:104:ARG:HB2	1:B:123:THR:O	1.97	0.64
1:B:13[B]:MET:HG2	1:B:14:VAL:N	2.12	0.64
1:B:26:ILE:HD13	1:B:26:ILE:O	1.98	0.63
1:B:103:ARG:HG3	1:B:104:ARG:N	2.12	0.63
1:B:103:ARG:NE	1:B:124:ASN:HB3	2.13	0.62
1:B:117:SER:OG	2:B:130:T33:I3'	2.86	0.61
1:B:13[B]:MET:HE2	1:B:54:GLU:HG2	1.83	0.61
1:B:15:LYS:HE2	1:B:17:LEU:HD21	1.84	0.60
1:B:13[B]:MET:CE	1:B:54:GLU:CG	2.81	0.56
1:B:104:ARG:HH11	1:B:104:ARG:HG3	1.71	0.56
1:B:98:ASN:O	1:B:101:GLY:O	2.24	0.56
1:B:26:ILE:HB	1:B:50:SER:O	2.06	0.55
1:B:13[B]:MET:HE3	1:B:56:HIS:HE1	1.68	0.53
1:B:35:LYS:HD2	1:B:40:THR:O	2.10	0.52
1:B:13[B]:MET:HG2	1:B:14:VAL:H	1.75	0.52
1:A:66:GLU:HG2	3:A:175:HOH:O	2.10	0.51
1:A:26:ILE:HD13	1:A:51:GLU:HA	1.93	0.51
1:B:55:LEU:HD13	1:B:58:LEU:HD21	1.93	0.50
1:A:39:ASP:O	1:A:39:ASP:CG	2.54	0.50
1:B:33:PHE:HB2	1:B:70:LYS:HB3	1.92	0.50
1:B:80:LYS:HA	3:B:177:HOH:O	2.11	0.50
1:A:36:ALA:HB2	1:A:42:GLU:CD	2.38	0.48
1:B:26:ILE:HG23	1:B:26:ILE:HD12	1.60	0.48
1:B:23:SER:HB2	1:B:24:PRO:HD2	1.96	0.47
1:B:42:GLU:HA	1:B:43:PRO:HD3	1.74	0.47
1:A:60:THR:OG1	1:A:63[B]:GLN:HG3	2.14	0.47
1:A:70:LYS:CD	1:A:92:GLU:HG3	2.44	0.47
1:B:66:GLU:OE2	1:B:98:ASN:OD1	2.32	0.47
1:B:12:LEU:C	1:B:13[A]:MET:HG3	2.40	0.47
1:A:11:PRO:HG2	1:A:59:THR:HG23	1.97	0.46
1:A:37:ALA:C	1:A:39:ASP:H	2.23	0.46
1:B:35:LYS:HD2	1:B:35:LYS:HA	1.75	0.45
1:A:18:ASP:C	1:A:18:ASP:OD1	2.61	0.44
1:A:46:SER:HB2	3:A:156:HOH:O	2.17	0.43
1:A:103:ARG:HH11	1:A:103:ARG:HD3	1.56	0.43
1:A:76:LYS:O	1:A:80:LYS:HG2	2.19	0.43
1:A:21:ARG:NH1	1:A:21:ARG:CG	2.71	0.43
1:A:38:ASP:OD1	1:A:38:ASP:N	2.50	0.42
1:B:34:ARG:NH2	1:B:66:GLU:O	2.53	0.42
1:B:90:HIS:C	1:B:90:HIS:CD2	2.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ALA:HB1	2:B:130:T33:C6	2.50	0.42
1:B:38:ASP:O	1:B:39:ASP:CB	2.62	0.42
1:A:103:ARG:HA	1:A:125:PRO:HD3	2.02	0.41
1:B:87:PHE:HB2	1:B:114:TYR:CD2	2.56	0.41
1:B:117:SER:C	2:B:130:T33:I3'	3.34	0.40
1:B:31:HIS:CE1	3:B:155:HOH:O	2.75	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%)	117 (98%)	2 (2%)	0	100	100
1	B	116/127 (91%)	107 (92%)	8 (7%)	1 (1%)	14	9
All	All	235/254 (92%)	224 (95%)	10 (4%)	1 (0%)	30	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	99	ASP

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%)	89 (87%)	13 (13%)	4	2
1	B	99/105 (94%)	86 (87%)	13 (13%)	4	2
All	All	201/210 (96%)	175 (87%)	26 (13%)	4	2

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	CYS
1	A	13[A]	MET
1	A	13[B]	MET
1	A	21	ARG
1	A	40	THR
1	A	46	SER
1	A	51	GLU
1	A	80	LYS
1	A	86	PRO
1	A	107	ILE
1	A	115	SER
1	A	117	SER
1	A	123	THR
1	B	26	ILE
1	B	27	ASN
1	B	35	LYS
1	B	38	ASP
1	B	39	ASP
1	B	42	GLU
1	B	55	LEU
1	B	56	HIS
1	B	76	LYS
1	B	82	LEU
1	B	104	ARG
1	B	117	SER
1	B	123	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	B	56	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	T33	B	130	-	22,23,23	1.39	4 (18%)	28,32,32	3.20	19 (67%)
2	T33	A	130	-	22,23,23	2.16	6 (27%)	28,32,32	5.09	22 (78%)

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	T33	B	130	-	-	4/12/12/12	0/2/2/2
2	T33	A	130	-	-	2/12/12/12	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	130	T33	C6'-C1'	5.75	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	130	T33	C3'-I3'	4.97	2.20	2.10
2	B	130	T33	C6'-C1'	3.31	1.44	1.38
2	B	130	T33	C4-C3	3.01	1.44	1.39
2	A	130	T33	O4-C1'	2.85	1.45	1.39
2	A	130	T33	C4-C3	2.65	1.43	1.39
2	A	130	T33	C5'-C4'	2.64	1.44	1.39
2	B	130	T33	C4'-C3'	2.40	1.44	1.39
2	B	130	T33	O4-C1'	2.16	1.44	1.39
2	A	130	T33	C7-C1	-2.09	1.46	1.51

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	130	T33	C5'-C6'-C1'	-13.14	104.72	119.73
2	A	130	T33	C2'-C3'-C4'	-11.40	107.87	120.55
2	A	130	T33	C1-C7-C8	8.07	130.64	114.13
2	A	130	T33	C5'-C4'-C3'	7.17	126.06	119.27
2	A	130	T33	C6'-C5'-C4'	6.77	127.26	120.50
2	B	130	T33	C5'-C6'-C1'	-6.68	112.10	119.73
2	B	130	T33	C2'-C3'-C4'	-6.44	113.38	120.55
2	A	130	T33	C6'-C1'-C2'	6.17	128.80	120.50
2	A	130	T33	C4'-C3'-I3'	5.65	125.20	119.76
2	A	130	T33	C7-C1-C6	5.41	130.97	120.90
2	B	130	T33	C4-O4-C1'	5.09	130.27	117.95
2	B	130	T33	C4'-C3'-I3'	4.63	124.22	119.76
2	A	130	T33	C2'-C3'-I3'	4.48	126.87	118.46
2	B	130	T33	O10-C9-O9	-4.29	114.34	124.08
2	A	130	T33	O4-C1'-C2'	-4.05	106.45	119.16
2	A	130	T33	C6-C1-C2	-4.03	112.99	118.55
2	B	130	T33	O4-C4-C5	3.83	130.78	120.74
2	A	130	T33	C4-O4-C1'	3.75	127.02	117.95
2	B	130	T33	C5'-C4'-C3'	3.75	122.81	119.27
2	A	130	T33	O4-C4-C5	3.71	130.46	120.74
2	A	130	T33	O10-C9-O9	-3.56	116.00	124.08
2	A	130	T33	C5-C4-C3	-3.49	114.78	120.20
2	B	130	T33	O4-C4-C3	-3.34	113.10	118.75
2	B	130	T33	C1-C7-C8	3.29	120.87	114.13
2	A	130	T33	O4'-C4'-C3'	-3.26	115.38	119.16
2	B	130	T33	C6-C1-C2	-3.20	114.13	118.55
2	B	130	T33	C6'-C1'-C2'	3.19	124.79	120.50
2	B	130	T33	O4'-C4'-C3'	-3.17	115.48	119.16
2	A	130	T33	C1'-C2'-C3'	3.11	125.26	119.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	130	T33	C7-C1-C6	3.01	126.50	120.90
2	B	130	T33	C6'-C5'-C4'	2.77	123.26	120.50
2	B	130	T33	C5-C6-C1	2.66	124.49	121.00
2	B	130	T33	C5-C4-C3	-2.64	116.10	120.20
2	A	130	T33	C7-C1-C2	-2.61	115.95	120.43
2	B	130	T33	O4-C1'-C2'	-2.46	111.46	119.16
2	A	130	T33	O4-C4-C3	-2.37	114.74	118.75
2	A	130	T33	C5-C6-C1	2.33	124.06	121.00
2	B	130	T33	C1'-C2'-C3'	2.28	123.62	119.14
2	A	130	T33	C1-C2-C3	2.24	124.55	120.45
2	A	130	T33	C4-C3-I3	2.11	123.61	120.24
2	B	130	T33	C2'-C3'-I3'	2.08	122.37	118.46

There are no chirality outliers.

All (6) torsion outliers are listed below:

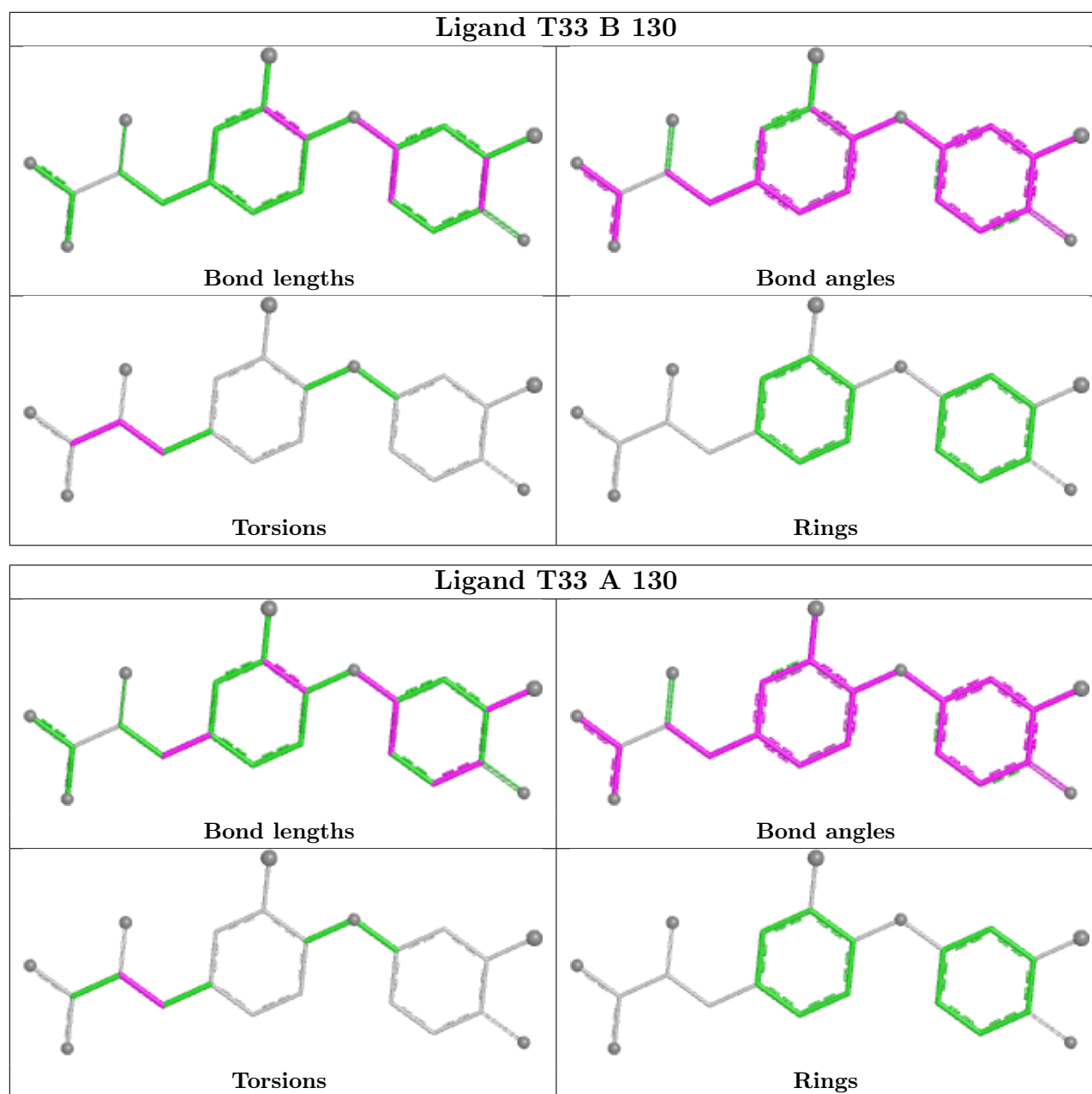
Mol	Chain	Res	Type	Atoms
2	A	130	T33	C1-C7-C8-N8
2	B	130	T33	C1-C7-C8-N8
2	B	130	T33	C1-C7-C8-C9
2	B	130	T33	N8-C8-C9-O10
2	A	130	T33	C1-C7-C8-C9
2	B	130	T33	N8-C8-C9-O9

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	130	T33	3	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.