



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:29 AM UTC

PDB ID : 1THC / pdb_00001thc
Title : CRYSTAL STRUCTURE DETERMINATION AT 2.3A OF HUMAN TRASTHYRETIN-3',5'-DIBROMO-2',4,4',6-TETRA-HYDROXYAURONE COMPLEX
Authors : Ciszak, E.; Cody, V.; Luft, J.R.
Deposited on : 1992-04-20
Resolution : 2.30 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

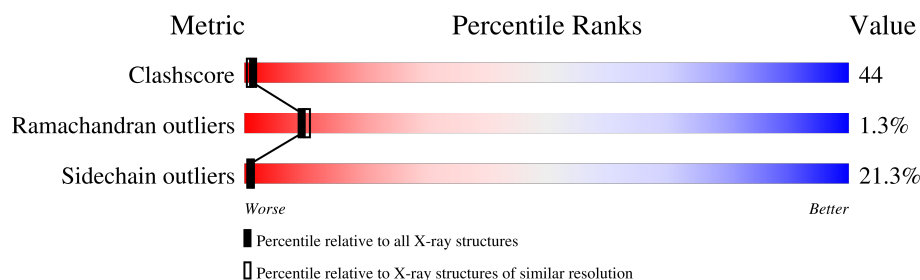
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	FL9	B	131	-	-	X	-

2 Entry composition [i](#)

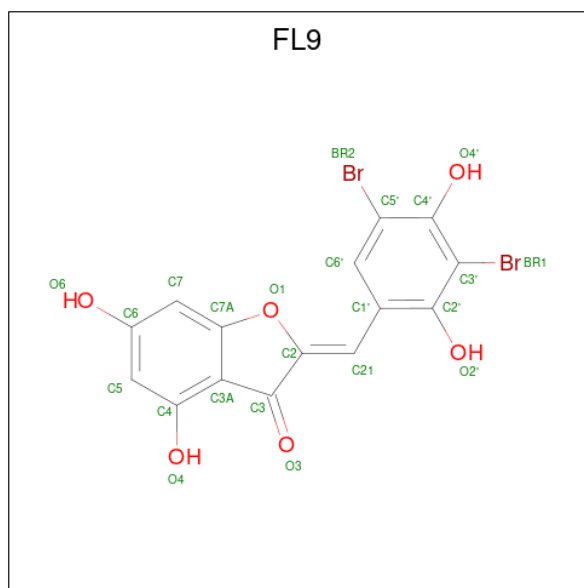
There are 3 unique types of molecules in this entry. The entry contains 1963 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	1	0
			909	581	149	177	2			
1	B	115	Total	C	N	O	S	0	1	0
			891	570	146	173	2			

- Molecule 2 is 3',5'-DIBROMO-2',4,4',6'-TETRAHYDROXY AURONE (CCD ID: FL9) (formula: C₁₅H₈Br₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	Br	C	O	0	0
			23	2	15	6		
2	A	1	Total	Br	C	O	0	0
			11	2	7	2		
2	B	1	Total	Br	C	O	0	0
			23	2	15	6		
2	B	1	Total	Br	C	O	0	0
			11	2	7	2		

- Molecule 3 is water.

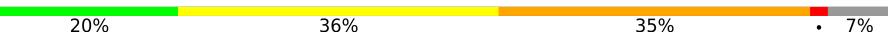
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total 47	O 47	0	0
3	B	48	Total 48	O 48	0	0

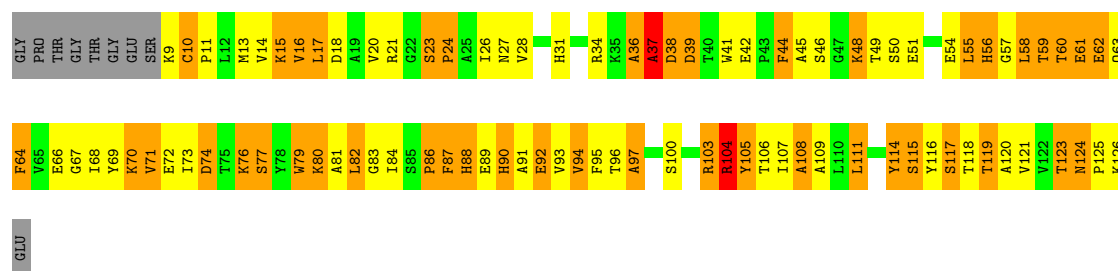
3 Residue-property plots

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.

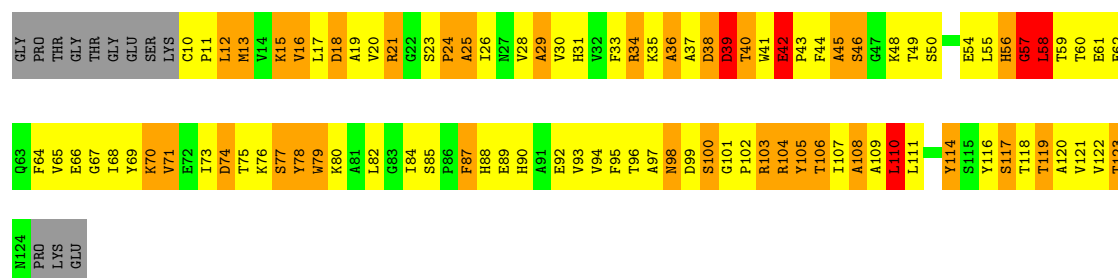
• Molecule 1: TRANSTHYRETIN

Chain A:  20% 36% 35% 7%



• Molecule 1: TRANSTHYRETIN

Chain B:  14% 46% 27% 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	43.40Å 85.84Å 65.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.179 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1963	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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: FL9

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	1.58	7/938 (0.7%)	3.37	161/1280 (12.6%)
1	B	1.48	2/918 (0.2%)	3.41	149/1252 (11.9%)
All	All	1.53	9/1856 (0.5%)	3.39	310/2532 (12.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	89	GLU	C-N	-6.27	1.26	1.33
1	A	111	LEU	C-O	-5.46	1.17	1.24
1	A	73	ILE	C-N	-5.39	1.26	1.33
1	B	58	LEU	N-CA	-5.32	1.39	1.46
1	A	20	VAL	C-N	-5.29	1.26	1.33
1	B	17	LEU	N-CA	5.27	1.52	1.45
1	A	79	TRP	C-N	-5.23	1.26	1.33
1	A	26	ILE	C-O	5.21	1.31	1.24
1	A	21	ARG	N-CA	-5.13	1.39	1.46

All (310) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	21	ARG	CD-NE-CZ	23.58	157.41	124.40
1	A	20	VAL	CA-C-N	18.05	153.14	121.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	VAL	C-N-CA	18.05	153.14	121.92
1	B	15	LYS	CA-CB-CG	15.84	145.77	114.10
1	A	70	LYS	CA-C-O	-13.51	105.92	120.24
1	B	94	VAL	O-C-N	12.90	137.11	123.18
1	B	57	GLY	CA-C-N	12.84	146.07	121.54
1	B	57	GLY	C-N-CA	12.84	146.07	121.54
1	B	104	ARG	CD-NE-CZ	12.71	142.20	124.40
1	B	30	VAL	CA-C-O	-12.58	107.56	120.27
1	B	93	VAL	CA-C-O	-12.43	105.24	120.78
1	B	105	TYR	CA-C-N	11.87	139.96	122.39
1	B	105	TYR	C-N-CA	11.87	139.96	122.39
1	A	90	HIS	CA-C-N	11.57	139.09	122.77
1	A	90	HIS	C-N-CA	11.57	139.09	122.77
1	A	97	ALA	CA-C-N	11.43	143.37	121.54
1	A	97	ALA	C-N-CA	11.43	143.37	121.54
1	B	117	SER	N-CA-CB	-11.25	94.18	111.05
1	B	77	SER	O-C-N	11.22	134.94	122.15
1	A	50	SER	CA-C-N	11.13	136.64	120.38
1	A	50	SER	C-N-CA	11.13	136.64	120.38
1	B	70	LYS	CA-C-N	-11.01	109.05	122.93
1	B	70	LYS	C-N-CA	-11.01	109.05	122.93
1	B	59	THR	CA-C-N	10.65	138.52	122.65
1	B	59	THR	C-N-CA	10.65	138.52	122.65
1	A	23	SER	N-CA-C	10.60	117.50	108.07
1	B	121	VAL	N-CA-CB	10.49	125.12	111.90
1	A	88	HIS	CA-CB-CG	10.37	124.17	113.80
1	B	25	ALA	CB-CA-C	10.28	127.38	110.22
1	A	70	LYS	O-C-N	10.15	135.15	123.27
1	A	64	PHE	CA-CB-CG	9.87	123.67	113.80
1	A	39	ASP	CA-CB-CG	-9.80	102.80	112.60
1	A	38	ASP	CA-CB-CG	-9.75	102.85	112.60
1	B	67	GLY	CA-C-N	9.74	134.55	122.37
1	B	67	GLY	C-N-CA	9.74	134.55	122.37
1	A	57	GLY	CA-C-N	9.62	133.35	120.65
1	A	57	GLY	C-N-CA	9.62	133.35	120.65
1	A	108	ALA	CA-C-O	-9.52	110.35	121.11
1	B	109	ALA	CA-C-O	-9.52	110.15	120.24
1	A	82	LEU	CB-CA-C	9.41	126.18	111.02
1	A	18	ASP	CA-CB-CG	9.35	121.95	112.60
1	A	14	VAL	CA-C-N	9.28	136.04	122.86
1	A	14	VAL	C-N-CA	9.28	136.04	122.86
1	B	46	SER	CA-C-O	-9.23	111.59	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	PHE	O-C-N	9.11	134.47	123.36
1	B	101	GLY	N-CA-C	-8.99	94.01	112.34
1	B	110	LEU	CA-C-O	-8.90	110.53	120.32
1	A	114	TYR	CA-CB-CG	-8.81	98.04	113.90
1	B	98	ASN	O-C-N	8.80	134.29	122.59
1	B	40	THR	CA-CB-OG1	-8.79	96.41	109.60
1	A	46	SER	N-CA-CB	8.71	126.64	111.39
1	B	56	HIS	CA-CB-CG	-8.63	105.17	113.80
1	A	71	VAL	CB-CA-C	8.58	122.51	110.84
1	B	82	LEU	N-CA-C	-8.57	101.81	113.30
1	B	17	LEU	CB-CA-C	8.55	125.11	109.71
1	A	60	THR	N-CA-CB	-8.54	95.64	111.53
1	A	89	GLU	CA-C-N	8.54	136.89	122.20
1	A	89	GLU	C-N-CA	8.54	136.89	122.20
1	B	101	GLY	O-C-N	8.47	130.24	121.77
1	A	51	GLU	CB-CG-CD	8.42	126.92	112.60
1	A	93	VAL	O-C-N	8.34	132.04	123.20
1	A	46	SER	CB-CA-C	-8.26	95.05	110.16
1	A	125	PRO	N-CA-C	-8.26	101.45	113.75
1	B	74	ASP	CA-CB-CG	-8.06	104.54	112.60
1	A	89	GLU	N-CA-CB	8.05	121.74	110.07
1	B	64	PHE	CA-C-N	8.02	130.85	122.27
1	B	64	PHE	C-N-CA	8.02	130.85	122.27
1	B	98	ASN	CA-CB-CG	-7.98	104.62	112.60
1	A	103	ARG	CA-C-O	-7.91	112.32	121.49
1	A	28	VAL	CA-C-O	-7.88	111.81	120.71
1	A	93	VAL	CA-C-O	-7.74	112.34	120.39
1	A	80	LYS	CA-C-O	7.72	128.65	120.70
1	A	71	VAL	O-C-N	-7.62	114.57	123.03
1	A	111	LEU	N-CA-C	7.61	121.84	109.59
1	A	103	ARG	O-C-N	7.58	133.20	122.74
1	B	71	VAL	CB-CA-C	7.57	121.14	110.84
1	B	12	LEU	CA-C-N	-7.54	110.97	122.81
1	B	12	LEU	C-N-CA	-7.54	110.97	122.81
1	B	100	SER	CA-C-O	7.53	128.60	120.55
1	A	26	ILE	O-C-N	7.52	131.56	122.83
1	B	71	VAL	O-C-N	-7.47	114.74	123.03
1	B	77	SER	CA-C-O	-7.42	112.56	120.42
1	A	42	GLU	CB-CG-CD	7.41	125.19	112.60
1	B	94	VAL	CA-C-O	-7.33	112.10	120.67
1	A	14	VAL	CA-C-O	-7.27	112.16	120.67
1	B	108	ALA	CA-C-N	7.26	133.01	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	108	ALA	C-N-CA	7.26	133.01	122.77
1	A	15	LYS	CA-C-N	7.21	132.13	123.19
1	A	15	LYS	C-N-CA	7.21	132.13	123.19
1	A	54	GLU	N-CA-C	7.18	121.55	110.42
1	A	62[A]	GLU	N-CA-C	7.15	122.39	112.45
1	A	62[B]	GLU	N-CA-C	7.15	122.39	112.45
1	B	77	SER	CB-CA-C	-7.14	98.71	110.85
1	B	80	LYS	CA-C-N	7.14	132.64	120.72
1	B	80	LYS	C-N-CA	7.14	132.64	120.72
1	A	67	GLY	O-C-N	7.11	131.12	123.58
1	B	121	VAL	O-C-N	7.11	130.60	122.99
1	B	123	THR	CA-C-N	7.11	134.49	121.70
1	B	123	THR	C-N-CA	7.11	134.49	121.70
1	B	100	SER	CA-C-N	7.09	133.00	121.87
1	B	100	SER	C-N-CA	7.09	133.00	121.87
1	B	101	GLY	CA-C-O	-7.08	111.40	121.52
1	A	73	ILE	CB-CG1-CD1	7.06	128.63	113.80
1	A	93	VAL	N-CA-CB	7.06	120.82	111.64
1	A	56	HIS	CB-CA-C	-7.04	97.02	110.24
1	B	43	PRO	O-C-N	7.01	131.79	122.89
1	B	20	VAL	N-CA-C	-6.95	105.06	111.67
1	A	114	TYR	CB-CA-C	-6.93	99.86	111.02
1	B	97	ALA	N-CA-C	-6.89	95.03	107.98
1	B	29	ALA	CB-CA-C	6.88	121.06	109.84
1	B	18	ASP	CB-CA-C	6.85	121.52	110.16
1	A	116	TYR	CA-C-N	-6.84	111.95	122.62
1	A	116	TYR	C-N-CA	-6.84	111.95	122.62
1	B	49	THR	N-CA-CB	6.82	120.13	109.83
1	A	31	HIS	CB-CA-C	-6.81	99.24	110.14
1	A	34	ARG	CA-C-O	-6.81	112.43	120.60
1	B	96	THR	N-CA-CB	6.76	121.18	110.57
1	B	75	THR	N-CA-C	6.76	120.74	112.23
1	A	31	HIS	CA-CB-CG	-6.74	107.06	113.80
1	A	68	ILE	CA-C-O	-6.71	113.27	120.59
1	A	51	GLU	CG-CD-OE1	6.71	133.83	118.40
1	A	44	PHE	CA-CB-CG	-6.69	107.11	113.80
1	B	122	VAL	N-CA-C	6.64	117.20	107.37
1	A	66	GLU	N-CA-CB	6.60	119.80	110.36
1	B	114	TYR	CA-C-O	-6.60	112.16	119.95
1	B	114	TYR	O-C-N	6.58	130.35	122.26
1	A	76	LYS	N-CA-CB	6.57	121.59	110.49
1	A	124	ASN	OD1-CG-ND2	6.57	129.17	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	123	THR	CA-CB-OG1	-6.55	99.77	109.60
1	B	42	GLU	CA-C-N	6.54	126.58	119.90
1	B	42	GLU	C-N-CA	6.54	126.58	119.90
1	B	71	VAL	CA-C-N	6.52	132.37	123.11
1	B	71	VAL	C-N-CA	6.52	132.37	123.11
1	A	120	ALA	CA-C-O	-6.50	113.68	120.70
1	B	117	SER	CA-C-N	-6.48	109.18	121.63
1	B	117	SER	C-N-CA	-6.48	109.18	121.63
1	A	69	TYR	O-C-N	6.47	131.61	123.19
1	A	87	PHE	O-C-N	-6.47	115.40	122.07
1	A	38	ASP	N-CA-C	6.44	120.40	112.54
1	B	13	MET	N-CA-CB	-6.41	100.11	111.08
1	B	16	VAL	O-C-N	6.38	129.82	123.18
1	A	121	VAL	CA-C-O	-6.34	114.09	120.31
1	A	84	ILE	CB-CA-C	-6.32	101.20	110.62
1	B	33	PHE	CA-C-O	-6.30	112.53	120.28
1	B	60	THR	CA-CB-CG2	6.30	121.22	110.50
1	B	50	SER	CA-C-N	6.30	133.57	121.54
1	B	50	SER	C-N-CA	6.30	133.57	121.54
1	B	21	ARG	CA-CB-CG	-6.29	101.51	114.10
1	B	111	LEU	O-C-N	6.27	131.19	123.10
1	B	36	ALA	CB-CA-C	6.27	120.14	109.80
1	A	93	VAL	CA-C-N	-6.26	114.98	123.12
1	A	93	VAL	C-N-CA	-6.26	114.98	123.12
1	A	109	ALA	CA-C-O	-6.25	113.39	120.32
1	B	24	PRO	CA-C-N	-6.25	113.87	122.30
1	B	24	PRO	C-N-CA	-6.25	113.87	122.30
1	B	16	VAL	CB-CA-C	6.23	118.83	110.42
1	A	117	SER	CB-CA-C	6.21	122.35	109.38
1	B	21	ARG	NE-CZ-NH1	-6.20	115.31	121.50
1	B	122	VAL	O-C-N	6.19	130.99	122.88
1	B	34	ARG	NE-CZ-NH2	6.18	124.76	119.20
1	B	94	VAL	N-CA-C	-6.17	99.59	108.48
1	B	21	ARG	NH1-CZ-NH2	6.17	127.32	119.30
1	A	51	GLU	O-C-N	-6.16	115.17	122.20
1	B	79	TRP	O-C-N	6.16	130.24	122.23
1	B	73	ILE	CA-C-O	-6.15	113.99	120.57
1	A	116	TYR	O-C-N	6.15	130.28	123.33
1	A	59	THR	CB-CA-C	-6.13	100.32	114.41
1	A	42	GLU	CA-C-N	6.12	127.49	119.84
1	A	42	GLU	C-N-CA	6.12	127.49	119.84
1	A	71	VAL	CA-C-N	6.10	131.42	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	VAL	C-N-CA	6.10	131.42	123.00
1	A	92	GLU	CA-CB-CG	6.08	126.25	114.10
1	A	37	ALA	CA-C-N	6.07	130.85	120.72
1	A	37	ALA	C-N-CA	6.07	130.85	120.72
1	B	75	THR	O-C-N	6.03	130.41	122.33
1	A	27	ASN	N-CA-CB	-6.01	103.05	112.13
1	B	62[A]	GLU	CB-CG-CD	6.00	122.81	112.60
1	B	62[B]	GLU	CB-CG-CD	6.00	122.81	112.60
1	A	31	HIS	O-C-N	5.96	130.24	123.27
1	B	106	THR	N-CA-CB	5.91	120.41	110.77
1	A	20	VAL	N-CA-CB	5.90	118.12	110.57
1	A	87	PHE	CA-C-O	5.90	127.01	120.82
1	A	88	HIS	CA-C-N	5.89	128.46	120.44
1	A	88	HIS	C-N-CA	5.89	128.46	120.44
1	A	119	THR	OG1-CB-CG2	-5.88	97.55	109.30
1	A	87	PHE	N-CA-C	5.87	117.36	111.07
1	A	10	CYS	N-CA-C	-5.87	101.99	110.08
1	B	29	ALA	N-CA-C	-5.85	100.45	109.76
1	B	64	PHE	CA-CB-CG	5.83	119.63	113.80
1	B	80	LYS	CA-C-O	5.83	126.60	120.42
1	B	88	HIS	CA-C-O	5.83	128.35	121.36
1	A	42	GLU	N-CA-C	5.83	117.89	109.04
1	B	21	ARG	CG-CD-NE	-5.81	99.23	112.00
1	A	104	ARG	NH1-CZ-NH2	-5.80	111.77	119.30
1	B	103	ARG	N-CA-C	5.80	123.14	110.80
1	A	10	CYS	CB-CA-C	5.75	118.53	109.27
1	A	123	THR	N-CA-CB	-5.75	102.05	111.66
1	B	78	TYR	CB-CA-C	5.74	120.61	110.85
1	A	38	ASP	N-CA-CB	-5.72	100.90	110.39
1	A	83	GLY	N-CA-C	5.72	123.49	115.43
1	B	26	ILE	CB-CA-C	5.71	119.49	110.81
1	A	62[A]	GLU	CB-CA-C	-5.70	99.34	110.11
1	A	62[B]	GLU	CB-CA-C	-5.70	99.34	110.11
1	A	104	ARG	N-CA-CB	5.70	119.54	110.65
1	B	108	ALA	O-C-N	-5.70	116.55	123.10
1	B	58	LEU	CA-C-N	-5.69	112.53	121.87
1	B	58	LEU	C-N-CA	-5.69	112.53	121.87
1	A	94	VAL	CB-CA-C	5.69	119.27	110.96
1	B	11	PRO	CB-CA-C	-5.68	102.94	110.27
1	A	88	HIS	N-CA-C	5.68	119.34	110.32
1	A	18	ASP	O-C-N	-5.67	116.58	123.27
1	A	27	ASN	O-C-N	-5.67	114.82	122.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	LEU	CA-C-O	-5.63	115.09	121.00
1	B	43	PRO	N-CA-CB	5.62	108.19	103.25
1	A	76	LYS	CG-CD-CE	5.61	124.21	111.30
1	B	94	VAL	CB-CA-C	-5.61	102.27	110.62
1	A	115	SER	CA-C-O	5.60	127.04	120.43
1	B	28	VAL	N-CA-C	-5.60	100.36	108.36
1	A	108	ALA	N-CA-CB	-5.59	101.52	111.08
1	A	37	ALA	CA-C-O	5.57	128.48	120.51
1	A	61	GLU	CA-C-N	5.57	133.51	121.64
1	A	61	GLU	C-N-CA	5.57	133.51	121.64
1	B	82	LEU	CA-CB-CG	5.57	135.80	116.30
1	A	114	TYR	CB-CG-CD1	-5.57	112.45	120.80
1	A	106	THR	CA-C-N	5.56	129.32	122.37
1	A	106	THR	C-N-CA	5.56	129.32	122.37
1	B	87	PHE	CA-C-O	5.56	126.78	120.00
1	A	56	HIS	CA-CB-CG	5.55	119.35	113.80
1	A	55	LEU	CA-C-O	5.54	127.74	120.15
1	B	104	ARG	NE-CZ-NH1	5.53	127.03	121.50
1	B	25	ALA	CA-C-O	5.53	126.62	120.43
1	B	65	VAL	O-C-N	-5.52	116.98	122.12
1	A	105	TYR	CA-C-O	5.51	126.39	120.38
1	A	57	GLY	CA-C-O	-5.51	112.41	119.13
1	B	40	THR	OG1-CB-CG2	5.51	120.32	109.30
1	A	77	SER	CA-C-N	5.51	127.66	120.28
1	A	77	SER	C-N-CA	5.51	127.66	120.28
1	A	49	THR	CA-C-O	5.51	127.80	121.47
1	B	120	ALA	N-CA-CB	5.51	120.41	110.83
1	A	27	ASN	CA-C-O	5.49	127.82	121.28
1	B	61	GLU	O-C-N	5.49	127.80	122.09
1	B	74	ASP	CB-CG-OD2	-5.48	105.79	118.40
1	B	116	TYR	N-CA-C	-5.47	100.75	109.07
1	B	78	TYR	CA-C-N	5.46	129.92	120.58
1	B	78	TYR	C-N-CA	5.46	129.92	120.58
1	A	15	LYS	O-C-N	-5.46	115.92	123.12
1	A	86	PRO	CB-CA-C	-5.45	103.08	110.60
1	B	76	LYS	CA-C-N	5.43	128.01	120.29
1	B	76	LYS	C-N-CA	5.43	128.01	120.29
1	B	54	GLU	CA-C-N	-5.43	114.57	122.44
1	B	54	GLU	C-N-CA	-5.43	114.57	122.44
1	A	90	HIS	CA-C-O	5.42	126.72	121.14
1	A	21	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	A	24	PRO	CB-CA-C	5.41	118.15	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	LYS	CA-C-O	-5.41	112.78	120.51
1	A	107	ILE	CB-CG1-CD1	-5.40	102.46	113.80
1	B	65	VAL	CA-CB-CG1	5.37	119.52	110.40
1	B	38	ASP	O-C-N	5.36	131.05	122.42
1	B	28	VAL	CB-CA-C	5.36	118.12	110.84
1	A	36	ALA	CB-CA-C	5.35	119.30	109.46
1	B	111	LEU	N-CA-CB	-5.34	102.63	110.85
1	A	121	VAL	N-CA-C	-5.33	98.29	107.24
1	B	49	THR	OG1-CB-CG2	5.32	119.94	109.30
1	B	102	PRO	N-CA-C	5.32	119.22	111.03
1	A	94	VAL	CA-C-N	-5.31	113.16	121.87
1	A	94	VAL	C-N-CA	-5.31	113.16	121.87
1	A	62[A]	GLU	CB-CG-CD	5.30	121.61	112.60
1	A	62[B]	GLU	CB-CG-CD	5.30	121.61	112.60
1	A	20	VAL	CA-C-O	-5.29	115.17	121.05
1	A	21	ARG	N-CA-C	5.28	120.00	113.50
1	A	44	PHE	N-CA-CB	-5.27	102.36	110.42
1	A	16	VAL	CA-C-O	5.26	126.06	120.48
1	A	48	LYS	N-CA-C	-5.25	101.20	109.50
1	B	116	TYR	CA-C-O	-5.24	115.67	121.33
1	B	11	PRO	CA-C-N	-5.23	114.86	122.44
1	B	11	PRO	C-N-CA	-5.23	114.86	122.44
1	B	80	LYS	CB-CA-C	5.21	119.70	110.85
1	B	87	PHE	CA-CB-CG	-5.18	108.62	113.80
1	A	59	THR	CA-CB-OG1	-5.17	101.85	109.60
1	A	61	GLU	O-C-N	5.16	128.09	122.20
1	B	15	LYS	CA-C-O	-5.15	114.21	120.54
1	A	15	LYS	CA-C-O	5.15	125.89	120.33
1	B	39	ASP	CA-C-O	5.15	127.81	121.84
1	A	118	THR	CA-C-N	5.13	130.64	122.59
1	A	118	THR	C-N-CA	5.13	130.64	122.59
1	A	17	LEU	CD1-CG-CD2	-5.12	99.55	110.80
1	B	38	ASP	N-CA-C	-5.11	107.07	113.15
1	B	16	VAL	CA-C-N	-5.11	113.93	122.92
1	B	16	VAL	C-N-CA	-5.11	113.93	122.92
1	A	72	GLU	CA-C-O	-5.11	114.81	120.38
1	A	55	LEU	CB-CG-CD2	-5.10	95.39	110.70
1	B	97	ALA	N-CA-CB	-5.08	102.97	110.49
1	A	107	ILE	N-CA-CB	-5.08	105.21	111.00
1	A	100	SER	CA-CB-OG	5.07	121.23	111.10
1	A	123	THR	OG1-CB-CG2	5.07	119.43	109.30
1	A	84	ILE	CB-CG1-CD1	5.06	124.43	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	85	SER	N-CA-CB	-5.06	101.37	110.37
1	B	79	TRP	CA-C-N	5.05	127.45	120.29
1	B	79	TRP	C-N-CA	5.05	127.45	120.29
1	A	89	GLU	CA-C-O	-5.03	115.52	120.70
1	A	26	ILE	CB-CG1-CD1	-5.02	103.25	113.80
1	A	120	ALA	N-CA-CB	-5.02	102.09	110.83
1	B	100	SER	N-CA-C	-5.02	105.28	111.40
1	B	70	LYS	O-C-N	5.01	129.70	123.28
1	B	45	ALA	O-C-N	5.01	129.26	122.59
1	B	60	THR	CB-CA-C	5.01	117.89	109.48
1	A	74	ASP	CA-C-N	5.00	126.95	120.44
1	A	74	ASP	C-N-CA	5.00	126.95	120.44
1	A	60	THR	CA-CB-OG1	-5.00	102.09	109.60
1	A	68	ILE	O-C-N	5.00	129.57	122.97

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	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	909	0	875	76	0
1	B	891	0	862	88	0
2	A	34	0	6	6	0
2	B	34	0	5	12	0
3	A	47	0	0	2	0
3	B	48	0	0	4	0
All	All	1963	0	1748	160	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 44.

All (160) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:MET:HE3	1:A:56:HIS:CD2	1.75	1.21
1:A:119:THR:HG23	2:A:130:FL9:BR1	2.09	1.08
1:B:92:GLU:HB3	3:B:234:HOH:O	1.57	1.03
1:A:79:TRP:HB2	1:A:86:PRO:HG3	1.40	0.98
1:A:60:THR:HG22	1:A:63:GLN:HB3	1.51	0.92
1:A:79:TRP:CB	1:A:86:PRO:HG3	2.00	0.91
1:B:118:THR:O	1:B:119:THR:HG22	1.69	0.90
1:A:60:THR:HG22	1:A:63:GLN:CB	2.02	0.89
1:A:79:TRP:HB2	1:A:86:PRO:CG	2.04	0.86
1:B:15:LYS:NZ	2:B:131:FL9:C21	2.38	0.86
1:A:23:SER:HB2	1:A:24:PRO:HD2	1.56	0.85
1:B:23:SER:HB2	1:B:24:PRO:CD	2.06	0.85
1:B:119:THR:HG23	2:B:130:FL9:BR1	2.35	0.81
1:B:15:LYS:HZ1	2:B:131:FL9:C21	1.94	0.81
1:A:13:MET:HE3	1:A:56:HIS:NE2	1.96	0.80
1:B:103:ARG:HG3	1:B:104:ARG:H	1.48	0.79
1:B:10:CYS:N	1:B:104:ARG:NH2	2.34	0.76
1:A:13:MET:CE	1:A:56:HIS:CD2	2.66	0.74
1:A:13:MET:CE	1:A:56:HIS:NE2	2.52	0.73
1:A:115:SER:OG	1:B:119:THR:HG22	1.88	0.72
1:A:60:THR:CG2	1:A:63:GLN:H	2.03	0.72
1:B:35:LYS:HD2	1:B:39:ASP:HA	1.72	0.71
1:A:76:LYS:HE3	1:A:80:LYS:HE3	1.73	0.70
1:B:36:ALA:HB2	1:B:42:GLU:HG2	1.74	0.69
1:A:10:CYS:HB2	3:A:142:HOH:O	1.92	0.68
1:A:108:ALA:CB	2:A:130:FL9:O2'	2.42	0.68
1:A:44:PHE:CZ	1:A:59:THR:HG21	2.29	0.67
1:A:16:VAL:CG1	1:A:111:LEU:HD11	2.25	0.67
1:B:23:SER:CB	1:B:24:PRO:CD	2.71	0.67
1:B:23:SER:HB2	1:B:24:PRO:HD2	1.75	0.66
1:B:118:THR:C	1:B:119:THR:CG2	2.68	0.66
1:B:13:MET:HG3	1:B:56:HIS:HD2	1.61	0.66
1:B:118:THR:O	1:B:119:THR:CG2	2.42	0.66
1:A:103:ARG:HB2	1:A:105:TYR:CE1	2.31	0.66
1:B:15:LYS:HZ3	2:B:131:FL9:C21	2.08	0.65
1:A:108:ALA:HB3	2:A:130:FL9:O2'	1.98	0.64
1:A:9:LYS:O	1:A:104:ARG:NH1	2.31	0.64
1:B:15:LYS:NZ	2:B:131:FL9:C1'	2.60	0.64
1:B:104:ARG:HG2	3:B:191:HOH:O	1.97	0.64
1:A:95:PHE:HE2	1:A:97:ALA:HB2	1.63	0.64
1:B:34:ARG:HG3	1:B:69:TYR:CE2	2.34	0.62
1:A:60:THR:HG22	1:A:63:GLN:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:LEU:HD21	1:B:58:LEU:HD21	1.81	0.61
1:B:90:HIS:C	1:B:90:HIS:CD2	2.79	0.60
1:A:38:ASP:O	1:A:39:ASP:CB	2.49	0.60
1:B:19:ALA:HB2	1:B:110:LEU:HD22	1.84	0.60
1:B:13:MET:HG3	1:B:56:HIS:CD2	2.36	0.60
1:A:44:PHE:CE2	1:A:59:THR:CG2	2.84	0.60
1:A:23:SER:CB	1:A:24:PRO:HD2	2.22	0.59
1:A:36:ALA:C	1:A:38:ASP:N	2.57	0.59
1:A:95:PHE:CE2	1:A:97:ALA:HB2	2.38	0.59
1:A:17:LEU:HD11	2:A:131:FL9:BR2	2.58	0.59
1:A:115:SER:OG	1:B:119:THR:CG2	2.50	0.59
1:B:29:ALA:HB2	1:B:48:LYS:HE3	1.83	0.58
1:B:55:LEU:HD22	1:B:58:LEU:HD11	1.86	0.57
1:B:103:ARG:HG3	1:B:104:ARG:N	2.18	0.57
1:A:23:SER:HB2	1:A:24:PRO:CD	2.30	0.57
1:A:71:VAL:O	1:A:92:GLU:HA	2.04	0.57
1:B:18:ASP:OD2	1:B:78:TYR:OH	2.23	0.57
1:A:94:VAL:HG12	1:B:89:GLU:HB2	1.87	0.57
1:B:10:CYS:N	1:B:104:ARG:HH21	2.03	0.56
1:A:77:SER:O	1:A:81:ALA:HB2	2.04	0.56
1:B:15:LYS:HZ1	2:B:131:FL9:C1'	2.15	0.56
1:A:13:MET:HE3	1:A:56:HIS:HD2	1.58	0.56
1:B:108:ALA:HB3	2:B:130:FL9:O2'	2.05	0.56
1:A:60:THR:CG2	1:A:63:GLN:CB	2.80	0.56
1:A:87:PHE:HB2	1:A:114:TYR:CD2	2.41	0.56
1:B:58:LEU:H	1:B:58:LEU:HD23	1.70	0.56
1:A:74:ASP:OD2	1:A:77:SER:HB2	2.05	0.56
1:A:44:PHE:CE2	1:A:59:THR:HG23	2.42	0.55
1:B:87:PHE:HB2	1:B:114:TYR:CE2	2.42	0.55
1:A:11:PRO:HB2	1:A:64:PHE:CD2	2.42	0.55
1:A:87:PHE:HD2	1:A:88:HIS:CD2	2.25	0.55
1:B:79:TRP:CZ3	1:B:84:ILE:HD13	2.41	0.55
1:B:37:ALA:C	1:B:39:ASP:H	2.14	0.54
1:A:38:ASP:O	1:A:39:ASP:HB2	2.07	0.54
1:A:60:THR:HG23	1:A:63:GLN:H	1.73	0.53
1:A:36:ALA:C	1:A:38:ASP:H	2.17	0.52
1:B:103:ARG:HG3	1:B:123:THR:O	2.09	0.52
1:B:35:LYS:HD2	1:B:39:ASP:C	2.33	0.52
1:B:15:LYS:HE2	2:B:131:FL9:C1'	2.39	0.52
1:A:44:PHE:CE2	1:A:59:THR:HG21	2.44	0.52
1:A:36:ALA:O	1:A:38:ASP:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:LYS:HD2	1:B:39:ASP:CA	2.38	0.52
1:B:41:TRP:HH2	1:B:68:ILE:HG22	1.75	0.52
1:B:56:HIS:O	1:B:57:GLY:C	2.51	0.52
1:B:71:VAL:HG23	1:B:95:PHE:HE1	1.75	0.52
1:B:55:LEU:CD2	1:B:58:LEU:HD21	2.40	0.52
1:B:118:THR:C	1:B:119:THR:HG22	2.33	0.52
1:A:48:LYS:NZ	3:A:151:HOH:O	2.32	0.51
1:A:15:LYS:O	1:A:108:ALA:HA	2.11	0.51
1:B:39:ASP:CG	1:B:39:ASP:O	2.52	0.51
1:A:60:THR:CG2	1:A:63:GLN:HB2	2.41	0.51
1:A:44:PHE:HZ	1:A:59:THR:HG21	1.74	0.50
1:A:82:LEU:HD12	1:A:82:LEU:O	2.12	0.49
1:B:15:LYS:C	1:B:16:VAL:HG23	2.36	0.49
1:A:36:ALA:O	1:A:37:ALA:C	2.54	0.49
1:A:61:GLU:HB3	1:A:62[B]:GLU:OE1	2.13	0.49
1:B:15:LYS:CE	2:B:131:FL9:C1'	2.91	0.49
1:B:108:ALA:CB	2:B:130:FL9:O2'	2.61	0.49
1:A:87:PHE:HB2	1:A:114:TYR:CE2	2.48	0.49
1:A:60:THR:HG23	1:A:62[A]:GLU:HB2	1.95	0.48
1:B:103:ARG:CG	1:B:104:ARG:H	2.22	0.48
1:A:87:PHE:CD2	1:A:88:HIS:CD2	3.01	0.48
1:B:18:ASP:OD2	1:B:21:ARG:NH1	2.38	0.48
1:B:10:CYS:N	1:B:104:ARG:HH22	2.10	0.48
1:B:31:HIS:CD2	1:B:46:SER:HB2	2.49	0.48
1:B:117:SER:O	1:B:118:THR:HB	2.14	0.48
1:B:15:LYS:C	1:B:16:VAL:CG2	2.86	0.47
1:B:79:TRP:CZ3	1:B:84:ILE:CD1	2.97	0.47
1:B:10:CYS:C	1:B:104:ARG:HH21	2.22	0.47
1:B:19:ALA:HB2	1:B:110:LEU:CD2	2.45	0.47
1:B:36:ALA:O	1:B:39:ASP:N	2.46	0.47
1:B:87:PHE:HB2	1:B:114:TYR:CD2	2.49	0.47
1:B:34:ARG:NH2	1:B:66:GLU:O	2.45	0.47
1:B:79:TRP:HA	1:B:79:TRP:CE3	2.50	0.47
1:B:35:LYS:HE2	1:B:41:TRP:CE2	2.49	0.46
1:B:107:ILE:HD12	1:B:107:ILE:N	2.31	0.46
1:A:103:ARG:HB2	1:A:105:TYR:CZ	2.51	0.45
1:B:23:SER:CB	1:B:24:PRO:HD3	2.45	0.45
1:B:44:PHE:O	1:B:45:ALA:HB2	2.14	0.45
1:B:15:LYS:CE	2:B:131:FL9:C6'	2.94	0.45
1:A:79:TRP:HB2	1:A:86:PRO:HG2	1.96	0.45
1:A:92:GLU:OE1	1:B:92:GLU:OE1	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:TYR:CD1	1:B:105:TYR:N	2.84	0.45
1:A:13:MET:HA	1:A:55:LEU:O	2.17	0.45
1:A:119:THR:CG2	2:A:130:FL9:BR1	3.02	0.45
1:B:58:LEU:HD23	1:B:58:LEU:HA	1.56	0.45
1:B:103:ARG:CG	1:B:104:ARG:N	2.79	0.45
1:B:12:LEU:O	1:B:58:LEU:HD12	2.17	0.44
1:B:79:TRP:CE3	1:B:84:ILE:CD1	3.00	0.44
1:A:44:PHE:CZ	1:A:59:THR:CG2	2.97	0.44
1:A:77:SER:O	1:A:81:ALA:CB	2.65	0.44
1:B:74:ASP:OD2	1:B:77:SER:HB2	2.17	0.44
1:A:44:PHE:O	1:A:45:ALA:HB2	2.16	0.44
1:B:58:LEU:HB2	3:B:213:HOH:O	2.17	0.44
1:B:21:ARG:NH1	1:B:78:TYR:OH	2.51	0.43
1:B:37:ALA:C	1:B:39:ASP:N	2.75	0.43
1:A:58:LEU:HA	1:A:58:LEU:HD23	1.81	0.43
1:A:15:LYS:HE2	2:A:131:FL9:C6'	2.48	0.43
1:A:124:ASN:C	1:A:126:LYS:N	2.72	0.43
1:B:18:ASP:OD1	1:B:18:ASP:C	2.62	0.43
1:B:103:ARG:HD3	1:B:103:ARG:HA	1.76	0.43
1:A:59:THR:HG22	1:A:63:GLN:OE1	2.19	0.42
1:B:41:TRP:CH2	1:B:68:ILE:HG22	2.53	0.42
1:A:90:HIS:HB2	1:A:91:ALA:H	1.53	0.42
1:B:15:LYS:HE2	2:B:131:FL9:C6'	2.49	0.42
1:A:114:TYR:N	1:A:114:TYR:CD1	2.87	0.41
1:A:41:TRP:CD2	1:A:70:LYS:HE2	2.55	0.41
1:B:34:ARG:HD2	3:B:207:HOH:O	2.20	0.41
1:A:60:THR:CG2	1:A:63:GLN:N	2.79	0.41
1:B:25:ALA:HB1	1:B:78:TYR:CE2	2.55	0.41
1:A:11:PRO:HG3	1:A:61:GLU:HA	2.03	0.41
1:B:98:ASN:HB3	1:B:99:ASP:H	1.44	0.41
1:A:70:LYS:HD3	1:A:92:GLU:OE2	2.21	0.40
1:B:79:TRP:CE3	1:B:84:ILE:HD12	2.55	0.40
1:B:70:LYS:HE3	1:B:92:GLU:CD	2.46	0.40
1:A:60:THR:HG22	1:A:63:GLN:N	2.34	0.40
1:A:105:TYR:CD1	1:A:105:TYR:N	2.89	0.40
1:B:106:THR:C	1:B:107:ILE:HD12	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	117/127 (92%)	108 (92%)	8 (7%)	1 (1%)	14	17
1	B	114/127 (90%)	102 (90%)	10 (9%)	2 (2%)	6	6
All	All	231/254 (91%)	210 (91%)	18 (8%)	3 (1%)	9	10

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	58	LEU
1	A	37	ALA
1	B	57	GLY

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	11/105 (10%)	8 (73%)	3 (27%)	0	0
1	B	36/105 (34%)	29 (81%)	7 (19%)	1	1
All	All	47/210 (22%)	37 (79%)	10 (21%)	1	1

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	THR
1	A	117	SER
1	A	123	THR

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Mol	Chain	Res	Type
1	B	38	ASP
1	B	39	ASP
1	B	40	THR
1	B	42	GLU
1	B	100	SER
1	B	110	LEU
1	B	119	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

4 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	FL9	A	130	2	25,25,25	0.76	0	35,38,38	2.43	6 (17%)
2	FL9	A	131	2	11,11,25	1.01	1 (9%)	15,16,38	0.94	0
2	FL9	B	131	2	11,11,25	1.01	1 (9%)	15,16,38	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FL9	B	130	2	25,25,25	0.76	0	35,38,38	2.42	6 (17%)

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	FL9	A	130	2	-	1/4/16/16	0/3/3/3
2	FL9	A	131	2	-	-	0/1/1/3
2	FL9	B	131	2	-	-	0/1/1/3
2	FL9	B	130	2	-	3/4/16/16	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	131	FL9	C21-C1'	-2.18	1.46	1.51
2	B	131	FL9	C21-C1'	-2.15	1.47	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	130	FL9	C1'-C21-C2	-10.68	116.09	130.32
2	A	130	FL9	C1'-C21-C2	-10.67	116.09	130.32
2	B	130	FL9	O1-C2-C21	-6.20	119.07	124.39
2	A	130	FL9	O1-C2-C21	-6.17	119.10	124.39
2	A	130	FL9	C21-C2-C3	2.92	128.65	126.25
2	A	130	FL9	C7A-C3A-C3	2.89	108.14	106.93
2	B	130	FL9	C21-C2-C3	2.89	128.62	126.25
2	A	130	FL9	C7A-C7-C6	-2.78	114.61	118.98
2	B	130	FL9	C7A-C7-C6	-2.77	114.62	118.98
2	B	130	FL9	C7A-C3A-C3	2.76	108.08	106.93
2	A	130	FL9	C7-C6-C5	2.71	124.19	120.47
2	B	130	FL9	C7-C6-C5	2.69	124.17	120.47

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	130	FL9	C3-C2-C21-C1'
2	B	130	FL9	C3-C2-C21-C1'

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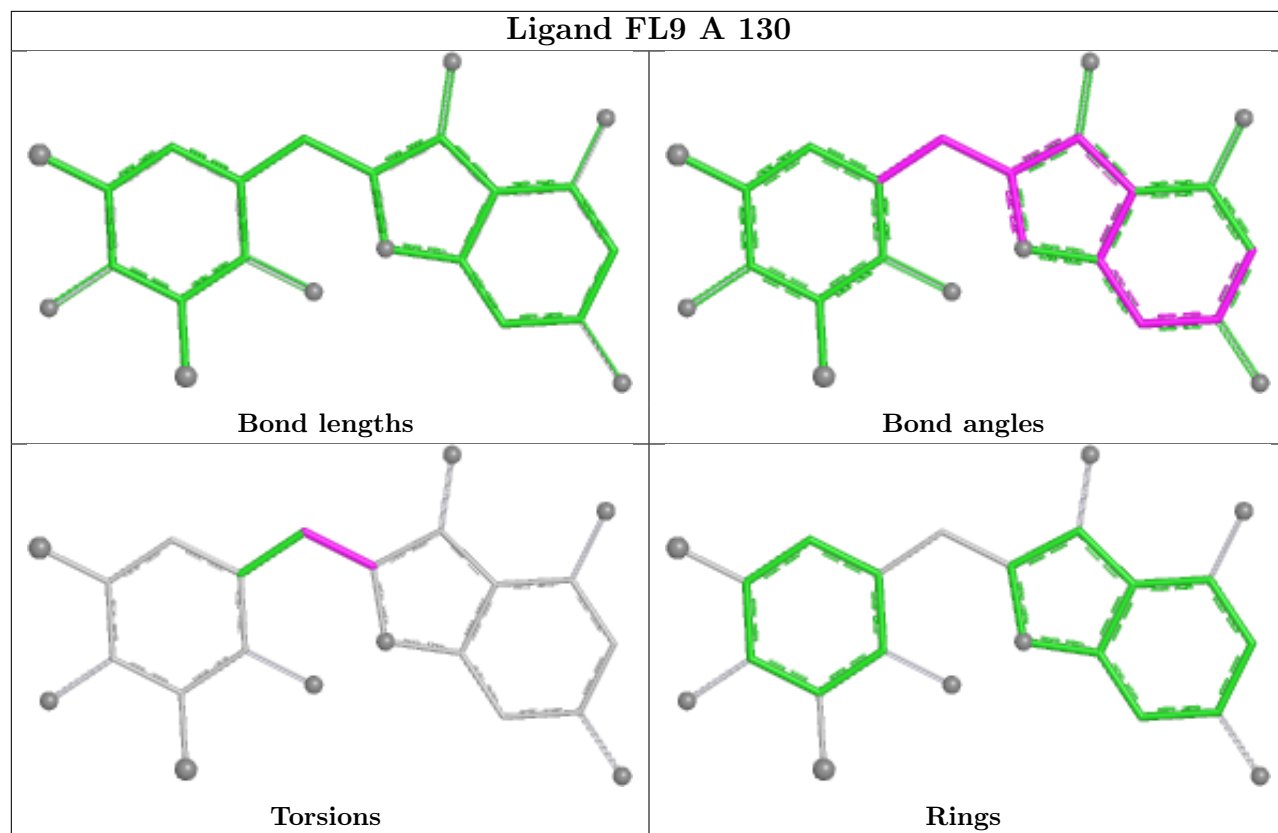
Mol	Chain	Res	Type	Atoms
2	B	130	FL9	C2'-C1'-C21-C2
2	B	130	FL9	C6'-C1'-C21-C2

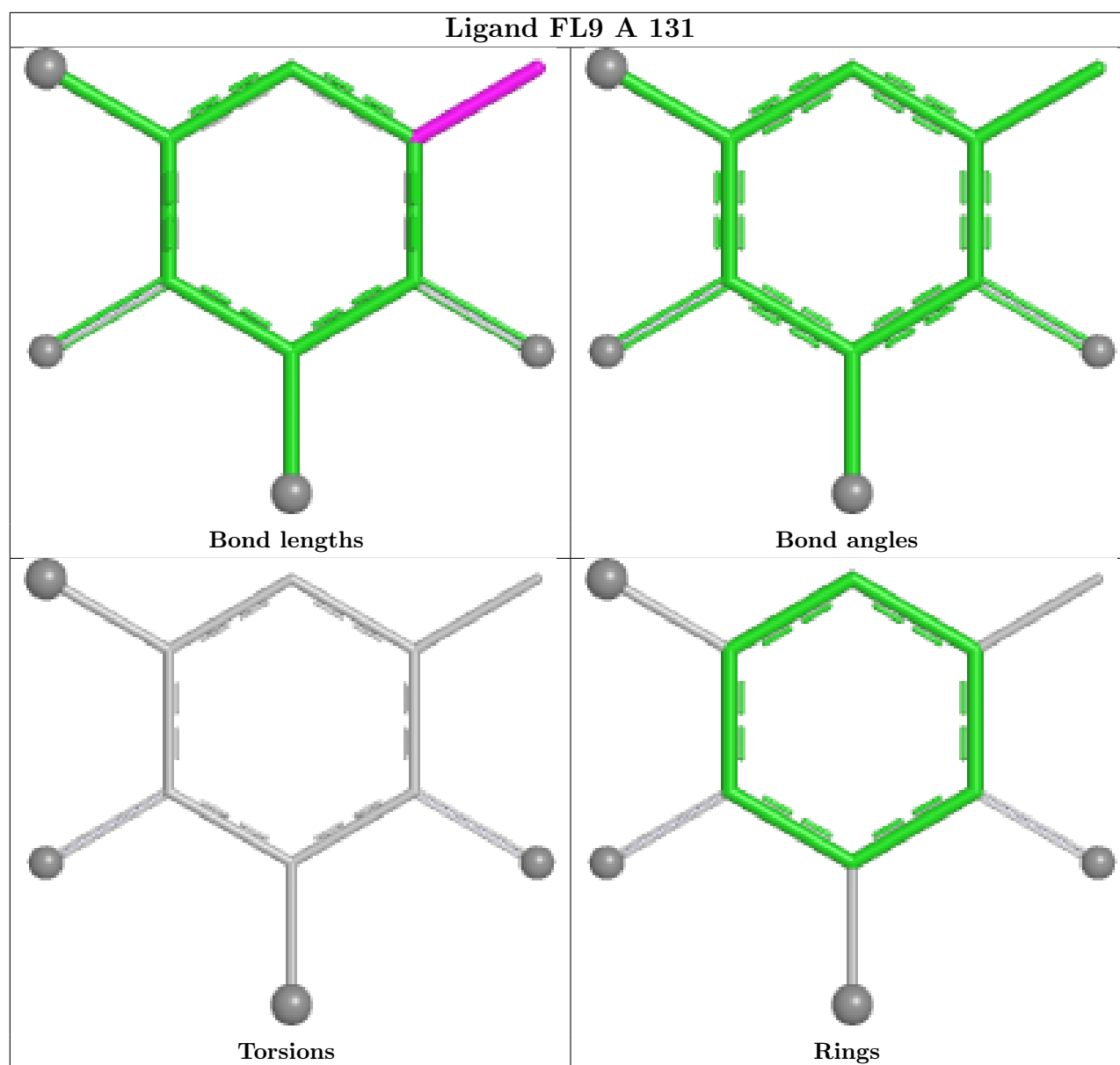
There are no ring outliers.

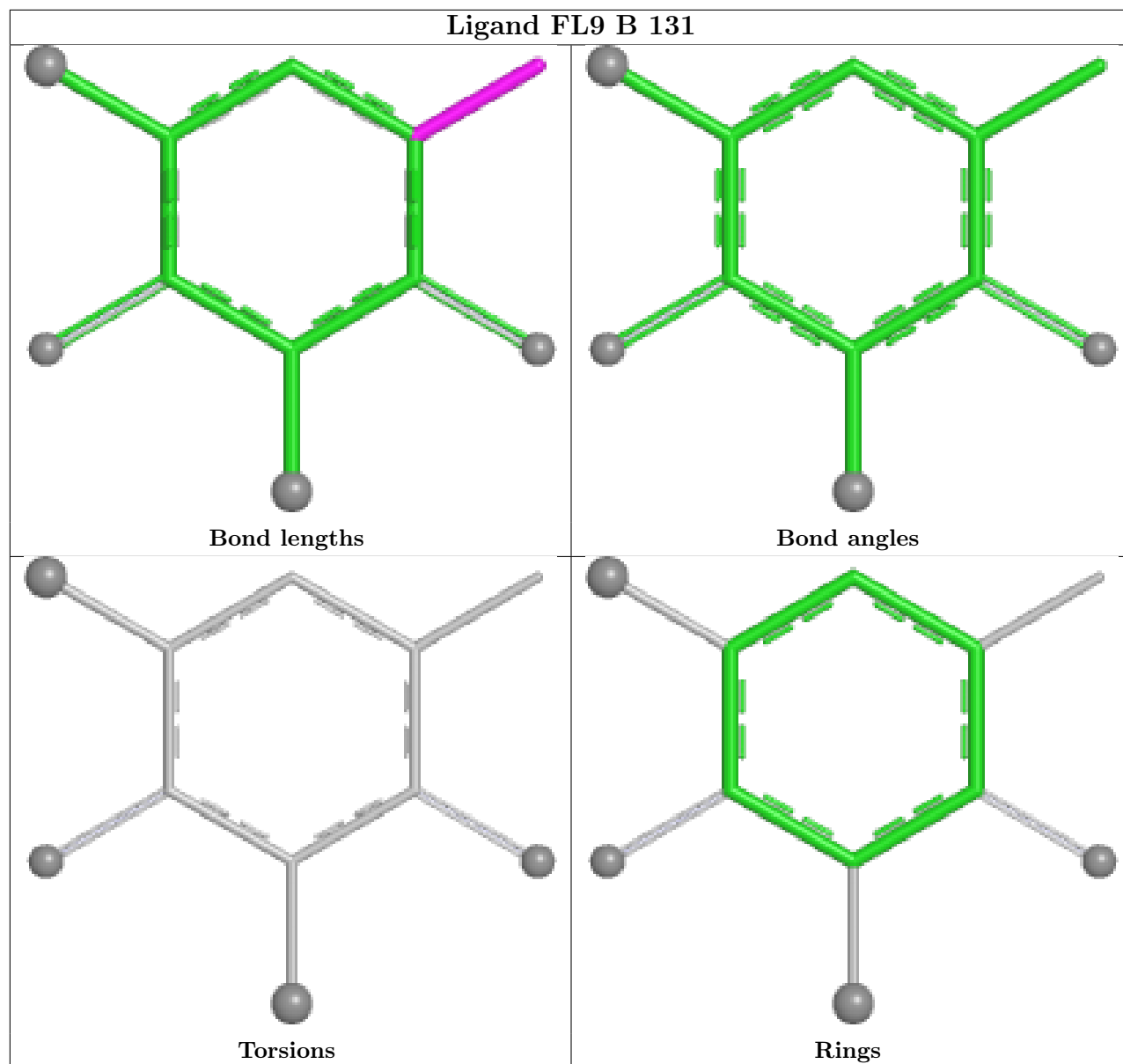
4 monomers are involved in 18 short contacts:

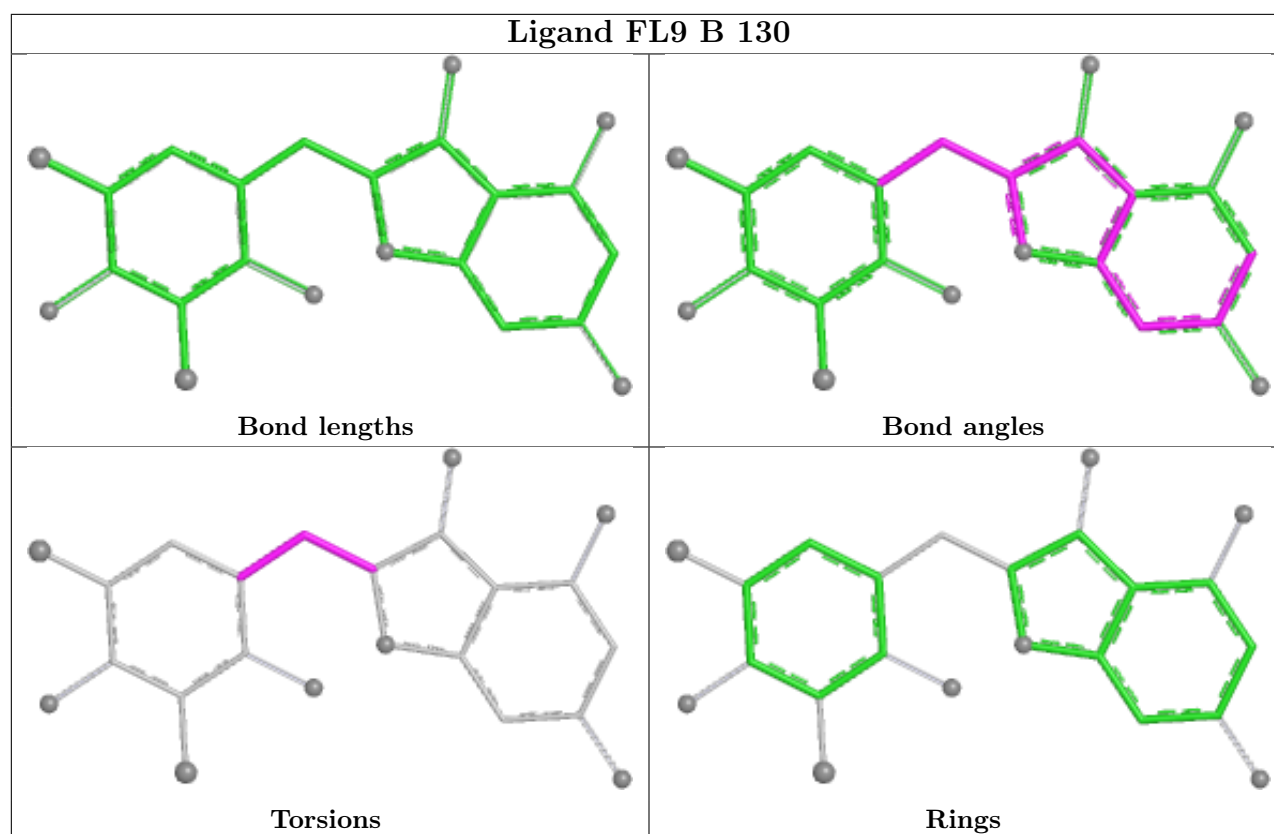
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	130	FL9	4	0
2	A	131	FL9	2	0
2	B	131	FL9	9	0
2	B	130	FL9	3	0

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.