



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:14 PM UTC

PDB ID : 1A2N / pdb_00001a2n
Title : STRUCTURE OF THE C115A MUTANT OF MURA COMPLEXED WITH
THE FLUORINATED ANALOG OF THE REACTION TETRAHEDRAL
INTERMEDIATE
Authors : Skarzynski, T.
Deposited on : 1998-01-06
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

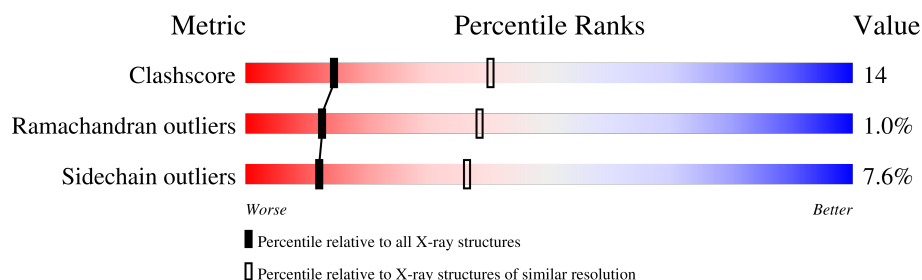
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	419	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3449 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.

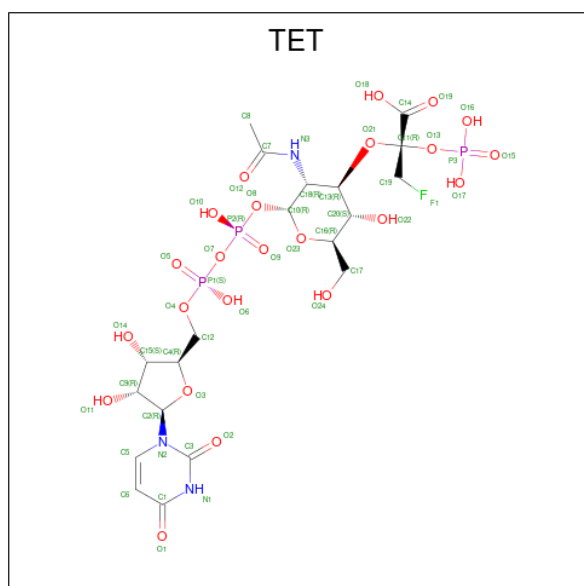
- Molecule 1 is a protein called UDP-N-ACETYLGLUCOSAMINE ENOLPYRUVYL TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	418	3128	1965	557	591	15	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	ALA	CYS	engineered mutation	UNP P0A749

- Molecule 2 is URIDINE-DIPHOSPHATE-2(N-ACETYLGLUCOSAMINYL-3-FLUORO-2-PHOSPHONOOXY)PROPIONIC ACID (CCD ID: TET) (formula: $C_{20}H_{31}FN_3O_{23}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	A	1	50	20	1	3	23	0	0

- Molecule 3 is water.

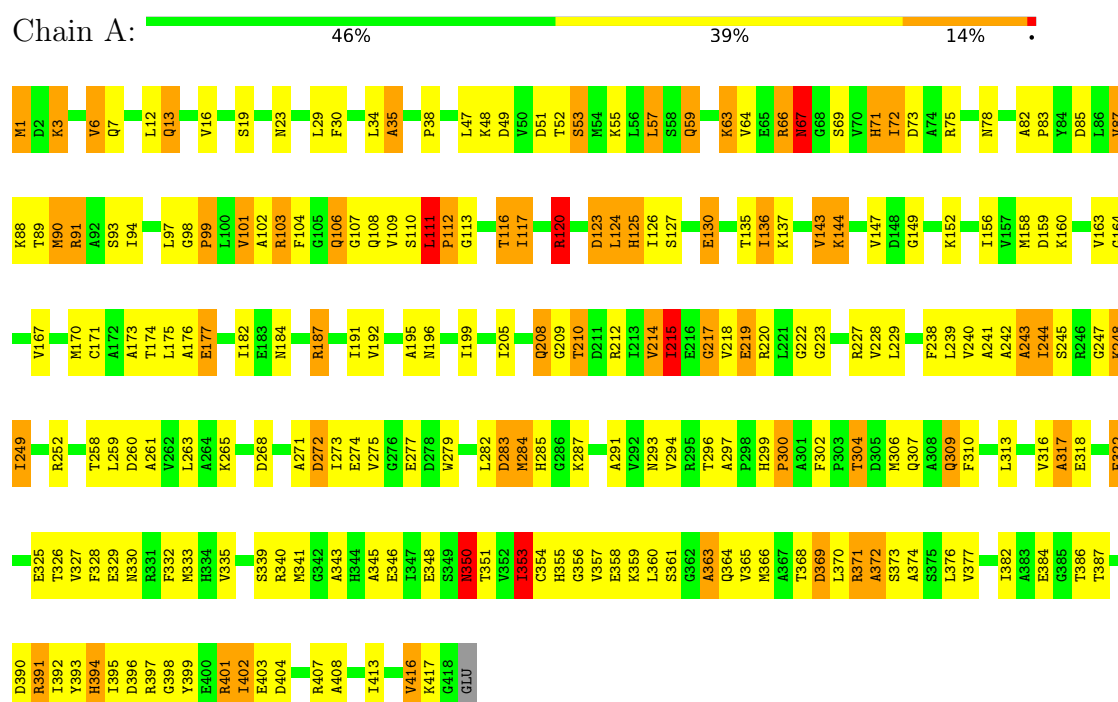
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	271	Total 271	O 271	0	0

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: UDP-N-ACETYLGLUCOSAMINE ENOLPYRUVYL TRANSFERASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	111.15Å 111.15Å 67.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.80	Depositor
% Data completeness (in resolution range)	99.2 (10.00-2.80)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR 3.1	Depositor
R, R_{free}	0.175 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3449	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: TET

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	1.37	16/3172 (0.5%)	2.42	217/4297 (5.1%)

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	1	2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	346	GLU	CA-CB	10.48	1.69	1.53
1	A	212	ARG	CA-C	-6.34	1.45	1.52
1	A	227	ARG	NE-CZ	6.00	1.39	1.33
1	A	346	GLU	CG-CD	5.88	1.66	1.52
1	A	394	HIS	CE1-NE2	5.78	1.38	1.32
1	A	355	HIS	CE1-NE2	5.63	1.38	1.32
1	A	67	ASN	CA-C	-5.60	1.45	1.52
1	A	294	VAL	CA-C	5.55	1.59	1.52
1	A	394	HIS	ND1-CE1	5.40	1.38	1.32
1	A	67	ASN	CA-CB	-5.34	1.44	1.53
1	A	360	LEU	CA-C	-5.32	1.46	1.52
1	A	355	HIS	ND1-CE1	5.21	1.37	1.32
1	A	71	HIS	ND1-CE1	5.17	1.37	1.32
1	A	285	HIS	ND1-CE1	5.15	1.37	1.32
1	A	252	ARG	NE-CZ	5.12	1.38	1.33
1	A	279	TRP	CD2-CE2	5.12	1.50	1.41

All (217) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	PRO	CA-C-N	-14.73	111.63	121.65
1	A	112	PRO	C-N-CA	-14.73	111.63	121.65
1	A	67	ASN	N-CA-CB	13.04	132.52	110.49
1	A	346	GLU	CB-CG-CD	10.42	130.32	112.60
1	A	66	ARG	N-CA-C	9.96	121.00	108.45
1	A	82	ALA	CA-C-O	9.94	128.61	119.76
1	A	215	ILE	CA-C-N	-9.76	109.25	122.72
1	A	215	ILE	C-N-CA	-9.76	109.25	122.72
1	A	353	ILE	CA-C-N	-9.20	109.80	122.77
1	A	353	ILE	C-N-CA	-9.20	109.80	122.77
1	A	91	ARG	CD-NE-CZ	-9.06	111.72	124.40
1	A	242	ALA	N-CA-C	9.02	122.29	111.82
1	A	350	ASN	N-CA-C	8.84	125.57	113.37
1	A	19	SER	CA-C-N	-8.48	112.28	120.34
1	A	19	SER	C-N-CA	-8.48	112.28	120.34
1	A	325	GLU	CA-C-N	-8.43	109.01	122.24
1	A	325	GLU	C-N-CA	-8.43	109.01	122.24
1	A	191	ILE	CA-CB-CG1	-8.34	96.22	110.40
1	A	346	GLU	CA-C-N	-8.31	109.20	122.50
1	A	346	GLU	C-N-CA	-8.31	109.20	122.50
1	A	350	ASN	CA-C-N	-8.31	110.88	122.93
1	A	350	ASN	C-N-CA	-8.31	110.88	122.93
1	A	67	ASN	CA-CB-CG	-8.30	104.30	112.60
1	A	19	SER	N-CA-C	8.25	121.17	110.53
1	A	346	GLU	CA-CB-CG	8.14	130.38	114.10
1	A	243	ALA	N-CA-C	8.02	119.80	111.14
1	A	85	ASP	N-CA-C	8.00	121.09	111.82
1	A	49	ASP	N-CA-C	7.96	119.95	111.28
1	A	354	CYS	CB-CA-C	-7.80	97.66	110.14
1	A	87	VAL	N-CA-C	7.77	122.92	112.04
1	A	363	ALA	N-CA-C	7.75	120.51	108.96
1	A	143	VAL	CB-CA-C	-7.75	100.41	111.19
1	A	364	GLN	CA-C-O	7.64	128.48	120.54
1	A	363	ALA	CA-C-N	-7.60	112.96	122.84
1	A	363	ALA	C-N-CA	-7.60	112.96	122.84
1	A	66	ARG	CB-CA-C	-7.57	95.69	113.02
1	A	215	ILE	CB-CA-C	-7.55	101.17	110.99
1	A	416	VAL	N-CA-C	7.55	118.74	108.17
1	A	327	VAL	N-CA-C	7.54	118.34	110.72
1	A	191	ILE	N-CA-C	7.50	117.58	110.53
1	A	171	CYS	N-CA-C	7.50	120.16	111.02
1	A	348	GLU	CB-CA-C	-7.43	99.77	110.62
1	A	120	ARG	CD-NE-CZ	7.34	134.68	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	MET	N-CA-C	7.33	120.36	108.34
1	A	16	VAL	CA-C-N	-7.21	111.42	122.09
1	A	16	VAL	C-N-CA	-7.21	111.42	122.09
1	A	277	GLU	N-CA-C	7.14	119.68	111.11
1	A	214	VAL	N-CA-C	7.12	118.07	108.11
1	A	268	ASP	CA-CB-CG	-7.10	105.50	112.60
1	A	247	GLY	CA-C-O	7.08	129.03	121.53
1	A	38	PRO	N-CA-C	7.05	122.29	111.15
1	A	287	LYS	N-CA-C	7.00	120.00	110.55
1	A	101	VAL	CB-CA-C	-6.84	102.78	112.22
1	A	340	ARG	CD-NE-CZ	-6.69	115.03	124.40
1	A	13	GLN	CB-CG-CD	-6.68	101.24	112.60
1	A	402	ILE	N-CA-C	6.67	119.42	111.09
1	A	310	PHE	CA-CB-CG	-6.66	107.14	113.80
1	A	318	GLU	CB-CG-CD	-6.66	101.29	112.60
1	A	377	VAL	N-CA-C	6.64	117.42	110.72
1	A	366	MET	CA-CB-CG	-6.61	100.89	114.10
1	A	69	SER	CA-C-N	-6.58	114.64	122.93
1	A	69	SER	C-N-CA	-6.58	114.64	122.93
1	A	360	LEU	CA-C-N	-6.58	112.36	122.09
1	A	360	LEU	C-N-CA	-6.58	112.36	122.09
1	A	397	ARG	N-CA-C	6.58	120.56	112.54
1	A	144	LYS	CA-C-N	-6.55	112.32	122.87
1	A	144	LYS	C-N-CA	-6.55	112.32	122.87
1	A	75	ARG	CA-C-N	-6.51	112.91	122.86
1	A	75	ARG	C-N-CA	-6.51	112.91	122.86
1	A	91	ARG	N-CA-CB	-6.45	98.58	110.32
1	A	223	GLY	CA-C-N	-6.45	113.44	121.83
1	A	223	GLY	C-N-CA	-6.45	113.44	121.83
1	A	30	PHE	N-CA-C	6.41	118.35	111.36
1	A	212	ARG	CB-CA-C	-6.38	101.30	110.62
1	A	187	ARG	N-CA-C	6.36	121.05	113.16
1	A	120	ARG	CB-CG-CD	6.35	125.91	111.30
1	A	177	GLU	CB-CG-CD	-6.35	101.81	112.60
1	A	159	ASP	N-CA-CB	-6.33	100.88	110.07
1	A	55	LYS	N-CA-C	6.25	118.90	111.33
1	A	72	ILE	N-CA-C	6.25	117.22	107.28
1	A	283	ASP	CA-CB-CG	-6.23	106.37	112.60
1	A	238	PHE	CA-CB-CG	-6.20	107.60	113.80
1	A	387	THR	CA-C-N	-6.18	114.87	123.10
1	A	387	THR	C-N-CA	-6.18	114.87	123.10
1	A	407	ARG	N-CA-C	6.15	118.95	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	ALA	N-CA-C	6.12	118.91	111.82
1	A	408	ALA	N-CA-C	6.11	119.83	112.38
1	A	364	GLN	CB-CA-C	6.09	120.53	110.78
1	A	51	ASP	N-CA-C	6.09	117.58	111.07
1	A	291	ALA	N-CA-C	6.08	119.18	110.24
1	A	52	THR	N-CA-C	6.04	118.36	111.11
1	A	101	VAL	N-CA-C	6.02	116.80	110.72
1	A	173	ALA	N-CA-C	6.00	123.58	110.80
1	A	343	ALA	N-CA-C	6.00	118.44	110.53
1	A	274	GLU	CA-C-N	-5.99	114.08	122.71
1	A	274	GLU	C-N-CA	-5.99	114.08	122.71
1	A	164	GLY	N-CA-C	5.95	119.87	112.73
1	A	217	GLY	CA-C-O	5.94	126.63	121.41
1	A	396	ASP	N-CA-C	5.91	119.58	112.38
1	A	369	ASP	N-CA-C	5.90	116.20	107.88
1	A	113	GLY	O-C-N	5.88	128.19	123.49
1	A	106	GLN	CA-CB-CG	-5.87	102.36	114.10
1	A	91	ARG	CA-CB-CG	5.86	125.81	114.10
1	A	124	LEU	CA-C-O	5.85	125.57	119.14
1	A	34	LEU	CA-C-N	-5.83	113.97	122.19
1	A	34	LEU	C-N-CA	-5.83	113.97	122.19
1	A	273	ILE	CB-CG1-CD1	-5.82	101.58	113.80
1	A	401	ARG	N-CA-C	5.79	119.54	111.90
1	A	167	VAL	N-CA-C	5.79	115.97	110.53
1	A	130	GLU	CA-C-N	-5.77	111.08	120.72
1	A	130	GLU	C-N-CA	-5.77	111.08	120.72
1	A	123	ASP	N-CA-C	5.74	123.03	110.80
1	A	249	ILE	CA-C-N	-5.73	115.63	123.14
1	A	249	ILE	C-N-CA	-5.73	115.63	123.14
1	A	284	MET	CA-C-O	5.73	126.45	119.11
1	A	127	SER	N-CA-C	5.69	117.48	111.28
1	A	277	GLU	CA-C-N	-5.69	113.52	122.79
1	A	277	GLU	C-N-CA	-5.69	113.52	122.79
1	A	332	PHE	CA-C-O	5.67	127.63	120.65
1	A	102	ALA	CA-C-O	5.67	126.49	119.97
1	A	371	ARG	CD-NE-CZ	-5.66	116.47	124.40
1	A	228	VAL	N-CA-C	5.63	116.86	109.21
1	A	340	ARG	CA-C-O	5.62	126.31	119.11
1	A	372	ALA	CB-CA-C	-5.62	101.41	110.74
1	A	239	LEU	N-CA-C	5.61	117.47	111.36
1	A	340	ARG	CA-C-N	-5.61	113.34	122.65
1	A	340	ARG	C-N-CA	-5.61	113.34	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	GLU	CG-CD-OE1	5.60	131.29	118.40
1	A	220	ARG	CA-C-N	-5.60	113.85	122.87
1	A	220	ARG	C-N-CA	-5.60	113.85	122.87
1	A	351	THR	CA-C-N	-5.57	115.77	122.90
1	A	351	THR	C-N-CA	-5.57	115.77	122.90
1	A	371	ARG	N-CA-C	5.54	117.31	111.28
1	A	219	GLU	CA-C-O	5.53	125.23	119.14
1	A	208	GLN	OE1-CD-NE2	-5.51	117.09	122.60
1	A	111	LEU	N-CA-CB	-5.51	99.60	109.68
1	A	403	GLU	N-CA-CB	-5.49	101.76	110.22
1	A	329	GLU	N-CA-C	5.49	119.29	112.59
1	A	67	ASN	CA-C-N	-5.49	113.43	120.34
1	A	67	ASN	C-N-CA	-5.49	113.43	120.34
1	A	191	ILE	N-CA-CB	-5.46	103.58	110.57
1	A	339	SER	N-CA-C	5.46	118.75	111.75
1	A	75	ARG	N-CA-C	5.46	117.99	111.71
1	A	273	ILE	N-CA-C	5.45	116.15	108.36
1	A	136	ILE	CA-C-N	-5.44	113.68	122.81
1	A	136	ILE	C-N-CA	-5.44	113.68	122.81
1	A	210	THR	N-CA-CB	5.43	118.68	110.42
1	A	258	THR	CB-CA-C	-5.43	100.70	110.37
1	A	272	ASP	CA-C-N	-5.42	116.10	122.93
1	A	272	ASP	C-N-CA	-5.42	116.10	122.93
1	A	369	ASP	CA-C-N	-5.42	113.50	120.65
1	A	369	ASP	C-N-CA	-5.42	113.50	120.65
1	A	307	GLN	N-CA-C	5.41	117.17	111.28
1	A	130	GLU	CB-CA-C	-5.41	101.82	110.79
1	A	317	ALA	CA-C-N	-5.40	113.94	121.99
1	A	317	ALA	C-N-CA	-5.40	113.94	121.99
1	A	245	SER	CA-C-O	5.39	126.20	119.78
1	A	391	ARG	CB-CG-CD	-5.38	98.92	111.30
1	A	7	GLN	CB-CA-C	-5.37	101.25	110.16
1	A	300	PRO	N-CA-CB	-5.36	96.70	102.60
1	A	373	SER	N-CA-C	5.36	117.12	111.28
1	A	394	HIS	CB-CG-CD2	-5.35	124.25	131.20
1	A	88	LYS	CA-C-O	5.35	125.94	119.31
1	A	184	ASN	CA-C-O	5.35	126.99	120.57
1	A	353	ILE	N-CA-C	5.35	115.95	108.89
1	A	218	VAL	CA-C-N	-5.34	112.67	121.92
1	A	218	VAL	C-N-CA	-5.34	112.67	121.92
1	A	78	ASN	CA-C-N	-5.31	113.12	121.62
1	A	78	ASN	C-N-CA	-5.31	113.12	121.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	VAL	CA-C-N	-5.30	114.09	119.98
1	A	163	VAL	C-N-CA	-5.30	114.09	119.98
1	A	53	SER	N-CA-C	5.29	117.73	111.33
1	A	159	ASP	N-CA-C	5.28	116.84	111.14
1	A	3	LYS	CA-C-N	-5.28	115.44	122.72
1	A	3	LYS	C-N-CA	-5.28	115.44	122.72
1	A	106	GLN	N-CA-C	5.28	116.82	108.96
1	A	120	ARG	NE-CZ-NH1	5.27	126.77	121.50
1	A	386	THR	CA-CB-CG2	5.26	119.44	110.50
1	A	391	ARG	CA-C-N	-5.25	112.52	121.97
1	A	391	ARG	C-N-CA	-5.25	112.52	121.97
1	A	135	THR	CA-C-O	5.25	126.08	120.46
1	A	265	LYS	N-CA-C	5.25	117.75	111.71
1	A	117	ILE	N-CA-C	5.24	120.25	109.34
1	A	363	ALA	CA-C-O	5.24	127.05	121.45
1	A	30	PHE	CA-CB-CG	-5.20	108.60	113.80
1	A	297	ALA	CA-C-N	-5.19	115.22	120.31
1	A	297	ALA	C-N-CA	-5.19	115.22	120.31
1	A	364	GLN	N-CA-C	5.19	117.07	108.20
1	A	335	VAL	CA-C-N	-5.18	114.28	119.56
1	A	335	VAL	C-N-CA	-5.18	114.28	119.56
1	A	35	ALA	CA-C-N	-5.16	114.54	122.60
1	A	35	ALA	C-N-CA	-5.16	114.54	122.60
1	A	107	GLY	CA-C-N	-5.16	114.95	122.44
1	A	107	GLY	C-N-CA	-5.16	114.95	122.44
1	A	346	GLU	N-CA-C	-5.16	100.76	109.07
1	A	284	MET	N-CA-C	5.13	119.39	113.18
1	A	271	ALA	CA-C-N	-5.13	115.72	122.85
1	A	271	ALA	C-N-CA	-5.13	115.72	122.85
1	A	174	THR	CA-C-N	-5.12	114.95	122.83
1	A	174	THR	C-N-CA	-5.12	114.95	122.83
1	A	346	GLU	OE1-CD-OE2	-5.12	110.62	122.90
1	A	326	THR	CB-CA-C	-5.11	100.44	109.02
1	A	244	ILE	CA-C-N	-5.11	114.51	122.73
1	A	244	ILE	C-N-CA	-5.11	114.51	122.73
1	A	404	ASP	CB-CA-C	-5.10	102.18	110.85
1	A	355	HIS	CA-CB-CG	-5.09	108.71	113.80
1	A	125	HIS	CA-C-O	5.08	126.33	121.00
1	A	322	PHE	CB-CA-C	-5.08	100.95	109.48
1	A	99	PRO	CA-C-N	-5.07	113.48	120.28
1	A	99	PRO	C-N-CA	-5.07	113.48	120.28
1	A	243	ALA	CA-C-O	5.06	125.92	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	HIS	N-CA-C	5.06	116.97	108.73
1	A	1	MET	CA-C-N	-5.05	113.53	120.71
1	A	1	MET	C-N-CA	-5.05	113.53	120.71
1	A	217	GLY	N-CA-C	5.05	117.26	111.36
1	A	265	LYS	CA-C-O	5.02	125.78	120.10
1	A	263	LEU	N-CA-C	5.01	117.40	111.33

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	67	ASN	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	ARG	Sidechain
1	A	187	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	3128	0	3209	87	0
2	A	50	0	26	5	0
3	A	271	0	0	7	1
All	All	3449	0	3235	90	1

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 14.

All (90) 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:116:THR:HG22	1:A:333:MET:HE1	1.29	1.08
1:A:111:LEU:HD13	1:A:143:VAL:HG22	1.62	0.80
1:A:64:VAL:HG22	1:A:72:ILE:HG12	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LEU:HG	1:A:371:ARG:HD3	1.69	0.74
1:A:116:THR:CG2	1:A:333:MET:HE1	2.13	0.72
1:A:243:ALA:HA	1:A:284:MET:HG3	1.73	0.71
1:A:116:THR:HG22	1:A:333:MET:CE	2.17	0.70
2:A:420:TET:O17	2:A:420:TET:H192	1.93	0.66
2:A:420:TET:O17	2:A:420:TET:C19	2.46	0.63
1:A:12:LEU:HD13	1:A:241:ALA:HB1	1.83	0.60
1:A:94:ILE:HA	1:A:109:VAL:HG11	1.84	0.59
1:A:152:LYS:HD2	1:A:177:GLU:HB3	1.84	0.57
2:A:420:TET:H9	3:A:555:HOH:O	2.04	0.57
1:A:35:ALA:HB1	1:A:222:GLY:O	2.06	0.55
1:A:47:LEU:HD13	1:A:398:GLY:HA2	1.89	0.55
1:A:87:VAL:HG13	1:A:93:SER:OG	2.07	0.54
1:A:176:ALA:O	1:A:217:GLY:HA3	2.07	0.54
1:A:316:VAL:HA	1:A:357:VAL:O	2.08	0.54
1:A:152:LYS:HD2	1:A:177:GLU:O	2.08	0.54
1:A:215:ILE:HD12	1:A:215:ILE:N	2.24	0.53
1:A:53:SER:HA	1:A:90:MET:HE1	1.92	0.52
1:A:195:ALA:HB3	1:A:208:GLN:HG3	1.90	0.52
1:A:365:VAL:HB	1:A:376:LEU:HD13	1.92	0.52
1:A:120:ARG:HA	2:A:420:TET:O11	2.10	0.52
1:A:341:MET:HG2	1:A:363:ALA:HB3	1.92	0.52
1:A:97:LEU:O	1:A:101:VAL:HG23	2.10	0.51
1:A:358:GLU:HA	3:A:640:HOH:O	2.10	0.51
1:A:120:ARG:HD2	1:A:328:PHE:CE1	2.46	0.51
1:A:293:ASN:ND2	1:A:322:PHE:H	2.09	0.51
1:A:98:GLY:HA3	3:A:632:HOH:O	2.11	0.50
1:A:120:ARG:HG2	3:A:555:HOH:O	2.11	0.50
1:A:350:ASN:N	1:A:350:ASN:HD22	2.11	0.49
1:A:374:ALA:HA	1:A:395:ILE:HD11	1.94	0.49
1:A:111:LEU:HD13	1:A:143:VAL:CG2	2.39	0.48
1:A:272:ASP:HB3	1:A:283:ASP:HB3	1.94	0.48
1:A:66:ARG:O	1:A:67:ASN:HB2	2.14	0.48
1:A:130:GLU:HG3	1:A:136:ILE:HD12	1.96	0.48
1:A:103:ARG:HG2	1:A:104:PHE:CE2	2.48	0.47
1:A:196:ASN:HA	1:A:199:ILE:HD12	1.96	0.47
1:A:57:LEU:HD23	1:A:72:ILE:HD13	1.95	0.47
1:A:192:VAL:HG22	1:A:209:GLY:N	2.30	0.47
1:A:63:LYS:HB2	1:A:73:ASP:HB3	1.96	0.47
1:A:244:ILE:HG22	1:A:313:LEU:HA	1.96	0.47
1:A:240:VAL:O	1:A:244:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ALA:HA	1:A:353:ILE:O	2.15	0.46
1:A:3:LYS:HE3	1:A:416:VAL:HG23	1.97	0.46
1:A:126:ILE:HG23	1:A:136:ILE:HD13	1.97	0.46
1:A:299:HIS:CG	1:A:300:PRO:HA	2.51	0.46
1:A:244:ILE:HD12	1:A:382:ILE:HD13	1.96	0.46
1:A:248:LYS:HE3	1:A:248:LYS:HB2	1.87	0.46
1:A:170:MET:SD	1:A:195:ALA:HB2	2.57	0.45
1:A:99:PRO:HD3	3:A:632:HOH:O	2.16	0.45
1:A:296:THR:HG21	1:A:304:THR:HA	1.97	0.45
1:A:3:LYS:HG2	1:A:390:ASP:HA	1.99	0.45
1:A:117:ILE:HA	1:A:330:ASN:O	2.16	0.45
1:A:47:LEU:O	1:A:48:LYS:C	2.60	0.44
1:A:284:MET:HB3	1:A:284:MET:HE3	1.80	0.44
1:A:6:VAL:HG13	1:A:413:ILE:HG12	1.99	0.44
1:A:64:VAL:HA	1:A:71:HIS:O	2.18	0.44
1:A:175:LEU:HD11	3:A:454:HOH:O	2.16	0.44
1:A:392:ILE:HD12	1:A:392:ILE:HA	1.64	0.44
1:A:259:LEU:O	1:A:260:ASP:C	2.60	0.44
1:A:399:TYR:HB3	1:A:402:ILE:HB	1.99	0.44
1:A:413:ILE:HG21	1:A:413:ILE:HD13	1.72	0.43
1:A:309:GLN:NE2	1:A:309:GLN:H	2.16	0.43
1:A:359:LYS:HE2	1:A:384:GLU:HB2	2.00	0.43
1:A:369:ASP:HA	1:A:394:HIS:CD2	2.53	0.43
1:A:392:ILE:O	1:A:393:TYR:C	2.61	0.43
1:A:1:MET:HE3	1:A:391:ARG:HH11	1.83	0.43
1:A:23:ASN:OD1	2:A:420:TET:H83	2.19	0.42
1:A:317:ALA:O	1:A:356:GLY:HA3	2.19	0.42
1:A:137:LYS:HG3	1:A:144:LYS:HB2	2.01	0.42
1:A:116:THR:HG21	1:A:368:THR:O	2.19	0.42
1:A:175:LEU:HD23	1:A:175:LEU:HA	1.86	0.42
1:A:306:MET:HE3	1:A:306:MET:HB3	1.77	0.42
1:A:147:VAL:HG13	1:A:149:GLY:O	2.20	0.42
1:A:111:LEU:HA	1:A:112:PRO:HD3	1.91	0.42
1:A:158:MET:HE2	1:A:158:MET:HB3	1.81	0.42
1:A:106:GLN:NE2	1:A:108:GLN:HE22	2.18	0.42
1:A:243:ALA:HA	1:A:284:MET:CG	2.48	0.41
1:A:125:HIS:CD2	1:A:125:HIS:H	2.38	0.41
1:A:156:ILE:O	1:A:182:ILE:HA	2.20	0.41
1:A:372:ALA:HB1	3:A:654:HOH:O	2.20	0.41
1:A:59:GLN:HG2	1:A:83:PRO:HG3	2.01	0.41
1:A:205:ILE:HA	1:A:214:VAL:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:ASN:HD22	1:A:350:ASN:H	1.68	0.41
1:A:244:ILE:CG2	1:A:313:LEU:HA	2.51	0.40
1:A:249:ILE:HD13	1:A:249:ILE:HG21	1.82	0.40
1:A:124:LEU:HD11	1:A:160:LYS:HG3	2.03	0.40
1:A:296:THR:HG22	1:A:302:PHE:HD1	1.86	0.40

All (1) 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)
3:A:467:HOH:O	3:A:643:HOH:O[1_554]	1.61	0.59

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	416/419 (99%)	389 (94%)	23 (6%)	4 (1%)	12	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	123	ASP
1	A	417	LYS
1	A	304	THR

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	329/331 (99%)	304 (92%)	25 (8%)	12	36

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	13	GLN
1	A	29	LEU
1	A	57	LEU
1	A	59	GLN
1	A	63	LYS
1	A	67	ASN
1	A	89	THR
1	A	91	ARG
1	A	103	ARG
1	A	110	SER
1	A	111	LEU
1	A	116	THR
1	A	210	THR
1	A	215	ILE
1	A	219	GLU
1	A	229	LEU
1	A	248	LYS
1	A	275	VAL
1	A	282	LEU
1	A	309	GLN
1	A	350	ASN
1	A	353	ILE
1	A	361	SER
1	A	401	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	13	GLN
1	A	42	GLN
1	A	59	GLN
1	A	67	ASN

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Mol	Chain	Res	Type
1	A	78	ASN
1	A	106	GLN
1	A	184	ASN
1	A	196	ASN
1	A	253	ASN
1	A	255	GLN
1	A	293	ASN
1	A	309	GLN
1	A	344	HIS
1	A	350	ASN
1	A	364	GLN
1	A	394	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	TET	A	420	-	49,52,52	2.64	16 (32%)	66,80,80	2.03	21 (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	TET	A	420	-	-	7/31/83/83	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	420	TET	P1-O7	-10.19	1.48	1.59
2	A	420	TET	P2-O7	-8.64	1.50	1.59
2	A	420	TET	C3-N1	-4.60	1.30	1.38
2	A	420	TET	C1-N1	-4.21	1.31	1.38
2	A	420	TET	P3-O13	-3.73	1.53	1.59
2	A	420	TET	O11-C9	3.20	1.50	1.43
2	A	420	TET	C11-C14	3.05	1.62	1.54
2	A	420	TET	O14-C15	2.91	1.50	1.43
2	A	420	TET	P3-O17	-2.81	1.44	1.54
2	A	420	TET	O21-C13	2.52	1.45	1.42
2	A	420	TET	P2-O9	-2.49	1.42	1.50
2	A	420	TET	P3-O15	-2.39	1.43	1.50
2	A	420	TET	O24-C17	2.34	1.52	1.42
2	A	420	TET	O22-C20	2.21	1.48	1.43
2	A	420	TET	O3-C4	-2.17	1.40	1.45
2	A	420	TET	C15-C4	2.11	1.58	1.53

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	420	TET	O22-C20-C13	6.29	126.07	109.94
2	A	420	TET	O11-C9-C15	4.97	127.73	111.82
2	A	420	TET	O13-P3-O15	-4.68	92.64	109.33
2	A	420	TET	N1-C3-N2	4.45	120.69	114.89
2	A	420	TET	O7-P1-O5	-3.78	99.34	110.70
2	A	420	TET	C13-C18-N3	-3.68	105.03	110.91
2	A	420	TET	O8-P2-O9	-3.09	99.94	109.81
2	A	420	TET	O14-C15-C4	3.06	119.88	111.08
2	A	420	TET	O14-C15-C9	-2.97	102.30	111.82
2	A	420	TET	O3-C2-N2	-2.59	102.49	108.36
2	A	420	TET	O12-C7-C8	2.55	126.60	122.05
2	A	420	TET	O6-P1-O7	2.55	114.17	107.27
2	A	420	TET	O22-C20-C16	-2.46	103.27	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	420	TET	O17-P3-O13	2.28	114.73	105.85
2	A	420	TET	O24-C17-C16	2.27	119.06	111.33
2	A	420	TET	O17-P3-O15	-2.21	102.23	110.83
2	A	420	TET	O23-C16-C17	2.20	111.89	106.44
2	A	420	TET	O17-P3-O16	2.17	115.94	107.80
2	A	420	TET	C6-C5-N2	-2.12	118.39	121.84
2	A	420	TET	O3-C4-C12	-2.01	102.89	109.33
2	A	420	TET	O16-P3-O13	2.00	113.65	105.85

There are no chirality outliers.

All (7) torsion outliers are listed below:

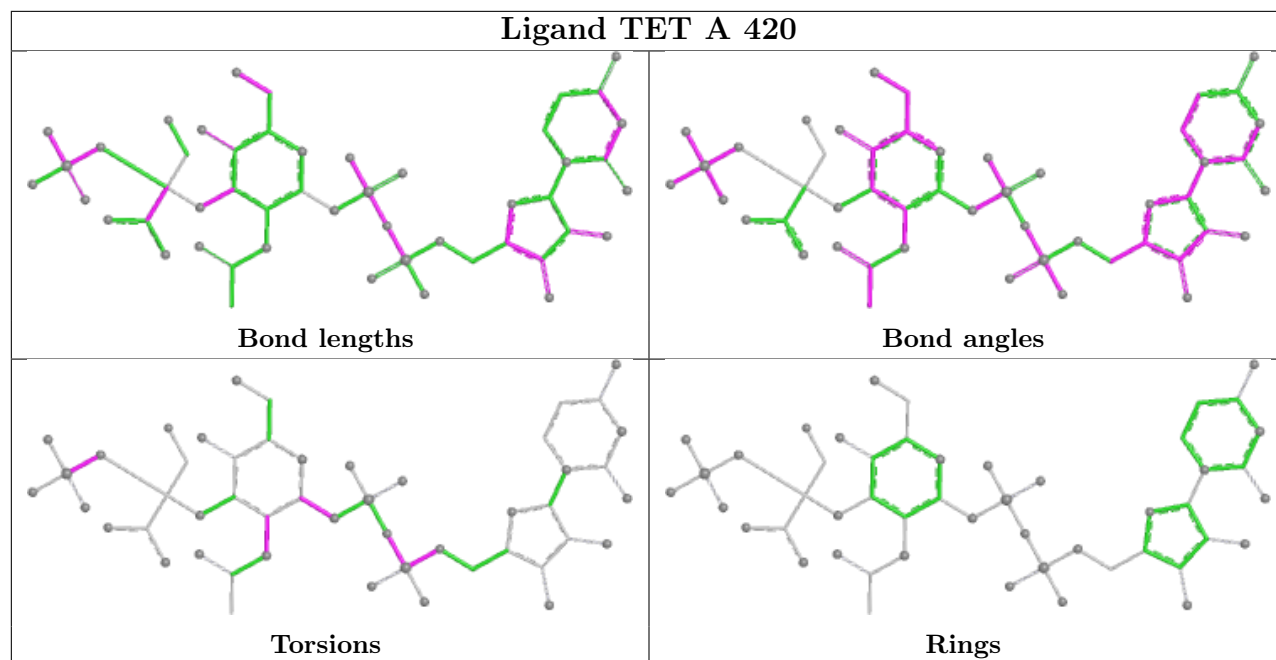
Mol	Chain	Res	Type	Atoms
2	A	420	TET	C12-O4-P1-O5
2	A	420	TET	C12-O4-P1-O6
2	A	420	TET	C12-O4-P1-O7
2	A	420	TET	O23-C10-O8-P2
2	A	420	TET	C11-O13-P3-O15
2	A	420	TET	P2-O7-P1-O5
2	A	420	TET	C13-C18-N3-C7

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	420	TET	5	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.