

# Full wwPDB X-ray Structure Validation Report (i)

May 22, 2020 – 05:49 pm BST

PDB ID : 1ELB

Title : Analogous inhibitors of elastase do not always bind analogously Authors : Mattos, C.; Rasmussen, B.; Ding, X.; Petsko, G.A.; Ringe, D.

Deposited on : 1993-12-07

Resolution : 2.10 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : NOT EXECUTED

EDS : NOT EXECUTED

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

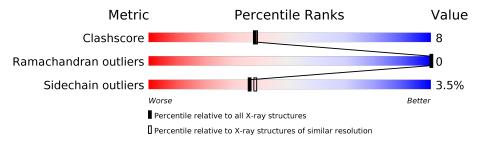
Validation Pipeline (wwPDB-VP) : 2.11

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$ 

The reported resolution of this entry is 2.10 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{resolution range}( ext{Å}))$
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain		
,		2.40			
1	Α	240	79%	18%	•



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 1987 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.

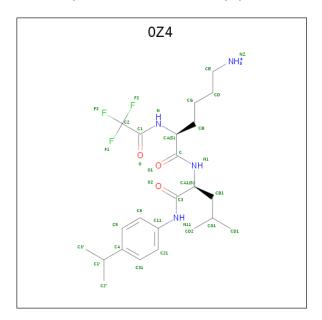
• Molecule 1 is a protein called ELASTASE.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Λ	240	Total	С	N	О	S	0	0	0
1	A	<u> </u>	1822	1135	330	347	10	0	U	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Modelled   Actual		Reference	
A	81	ASN	ASP	CONFLICT	UNP P00772	

• Molecule 2 is 6-ammonio-N-(trifluoroacetyl)-L-norleucyl-N-[4-(1-methylethyl)phenyl]-L-leuc inamide (three-letter code: 0Z4) (formula: C<sub>23</sub>H<sub>36</sub>F<sub>3</sub>N<sub>4</sub>O<sub>3</sub>).



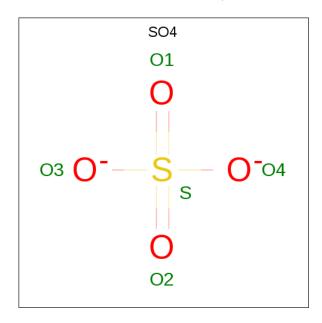
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	Λ	1	Total	С	F	N	О	0	0
	A	1	33	23	3	4	3	0	U

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).



Mo	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0

 $\bullet$  Molecule 4 is SULFATE ION (three-letter code: SO4) (formula:  $\mathrm{O_4S}).$ 



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	126	Total O 126 126	0	0

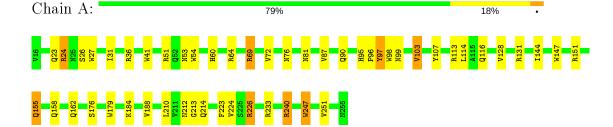


# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: ELASTASE





# 4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	50.69Å 58.05Å 75.25Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	10.00 - 2.10	Depositor	
% Data completeness	(Not available) (10.00-2.10)	Depositor	
(in resolution range)	(10.00 2.10)		
$R_{merge}$	(Not available)	Depositor	
$R_{sym}$	(Not available)	Depositor	
Refinement program	X-PLOR	Depositor	
$R, R_{free}$	0.150 , (Not available)	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	1987	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP	



# 5 Model quality (i)

### 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 0Z4, CA, SO4

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	Bo	ond angles
IVIOI	Chain	RMSZ	# Z >5	RMSZ	# Z  > 5
1	A	0.82	0/1862	1.53	41/2543 (1.6%)

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	240	ARG	NE-CZ-NH2	-13.16	113.72	120.30
1	$\frac{A}{A}$	27	TRP	CD1-CG-CD2	8.90	113.42	106.30
1	A	147	TRP	CD1-CG-CD2	8.45	113.06	106.30
1	A	240	ARG	NE-CZ-NH1	8.33	124.47	120.30
1	A	247	TRP	CD1-CG-CD2	8.30	112.94	106.30
1	A	41	TRP	CD1-CG-CD2	8.09	112.77	106.30
1	A	98	TRP	CE2-CD2-CG	-7.79	101.07	107.30
1	A	27	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	A	247	TRP	CE2-CD2-CG	-7.47	101.33	107.30
1	A	147	TRP	CE2-CD2-CG	-7.40	101.38	107.30
1	A	24	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	A	64	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	A	226	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	A	179	TRP	CD1-CG-CD2	7.12	112.00	106.30
1	A	247	TRP	CG-CD2-CE3	6.96	140.16	133.90
1	A	179	TRP	CE2-CD2-CG	-6.90	101.78	107.30
1	A	98	TRP	CD1-CG-CD2	6.81	111.75	106.30
1	A	41	TRP	CE2-CD2-CG	-6.68	101.95	107.30
1	A	54	TRP	CD1-CG-CD2	6.67	111.64	106.30
1	A	24	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	54	TRP	CE2-CD2-CG	-6.57	102.05	107.30
1	A	98	TRP	CG-CD2-CE3	6.10	139.39	133.90
1	A	27	TRP	CG-CD1-NE1	-6.01	104.09	110.10
1	A	131	ARG	NE-CZ-NH1	5.98	123.29	120.30



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Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
1	A	103	VAL	CB-CA-C	-5.88	100.23	111.40
1	A	27	TRP	CB-CG-CD1	-5.87	119.37	127.00
1	A	41	TRP	CG-CD1-NE1	-5.78	104.32	110.10
1	A	247	TRP	CB-CG-CD1	-5.78	119.49	127.00
1	A	97	TYR	CB-CG-CD2	-5.72	117.57	121.00
1	A	54	TRP	CG-CD2-CE3	5.63	138.97	133.90
1	A	147	TRP	CG-CD1-NE1	-5.61	104.49	110.10
1	A	240	ARG	CG-CD-NE	-5.50	100.24	111.80
1	A	98	TRP	CB-CG-CD1	-5.48	119.88	127.00
1	A	233	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	151	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	27	TRP	CG-CD2-CE3	5.34	138.70	133.90
1	A	247	TRP	CG-CD1-NE1	-5.30	104.80	110.10
1	A	147	TRP	CB-CG-CD1	-5.18	120.27	127.00
1	A	147	TRP	CG-CD2-CE3	5.13	138.52	133.90
1	A	69	ARG	CB-CA-C	-5.05	100.29	110.40
1	A	155	GLN	CA-CB-CG	5.03	124.47	113.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	1822	0	1759	27	14
2	A	33	0	36	11	0
3	A	1	0	0	0	0
4	A	5	0	0	0	0
5	A	126	0	0	3	4
All	All	1987	0	1795	28	14

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 8.

All (28) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
1:A:224:VAL:HG22	2:A:256:0Z4:HB21	1.58	0.86
1:A:223:PHE:HA	2:A:256:0Z4:HA1	1.61	0.80
1:A:224:VAL:HG13	2:A:256:0Z4:HD12	1.71	0.72
1:A:24:ARG:HH22	1:A:81:ASN:HD22	1.44	0.65
1:A:188:VAL:HG23	1:A:240:ARG:HG3	1.77	0.64
1:A:60:HIS:CD2	2:A:256:0Z4:HB3	2.33	0.62
1:A:87:VAL:HG23	1:A:116:GLN:NE2	2.18	0.58
1:A:31:ILE:HG22	1:A:72:VAL:HG12	1.87	0.56
2:A:256:0Z4:HG2	5:A:676:HOH:O	2.07	0.54
1:A:223:PHE:HB2	2:A:256:0Z4:HN11	1.72	0.54
1:A:226:ARG:HG2	2:A:256:0Z4:C31	2.39	0.53
1:A:24:ARG:HH22	1:A:81:ASN:ND2	2.05	0.52
1:A:90:GLN:HE22	1:A:113:ARG:NH1	2.08	0.52
1:A:60:HIS:CG	2:A:256:0Z4:HB3	2.45	0.52
1:A:247:TRP:O	1:A:251:VAL:HG23	2.11	0.50
1:A:188:VAL:CG2	1:A:240:ARG:HG3	2.42	0.50
1:A:226:ARG:HD3	2:A:256:0Z4:H3'2	1.96	0.48
1:A:226:ARG:HG2	2:A:256:0Z4:H3	1.96	0.47
1:A:184:LYS:N	1:A:184:LYS:HD2	2.31	0.46
1:A:223:PHE:HA	2:A:256:0Z4:HD23	1.98	0.46
1:A:144:ILE:O	1:A:162:GLN:HA	2.20	0.42
1:A:87:VAL:HG11	1:A:114:LEU:HD13	2.02	0.42
1:A:176:SER:HB2	5:A:590:HOH:O	2.19	0.42
1:A:97:TYR:HD2	1:A:107:TYR:CZ	2.38	0.42
1:A:24:ARG:HG3	5:A:624:HOH:O	2.20	0.42
1:A:23:GLN:HB2	1:A:26:SER:OG	2.20	0.41
1:A:76:ASN:HA	1:A:158:GLN:O	2.20	0.41
1:A:90:GLN:HE22	1:A:113:ARG:HH11	1.68	0.41

All (14) 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	$egin{aligned}  ext{Interatomic} \  ext{distance} \ ( ext{Å}) \end{aligned}$	Clash overlap (Å)
1:A:97:TYR:CE2	1:A:214:GLN:OE1[3_746]	1.35	0.85
1:A:97:TYR:CZ	1:A:214:GLN:OE1[3_746]	1.44	0.76
1:A:96:PRO:N	5:A:412:HOH:O[3_746]	1.58	0.62
1:A:96:PRO:CD	1:A:212:ASN:CB[3_746]	1.69	0.51
1:A:155:GLN:NE2	5:A:630:HOH:O[2_664]	1.77	0.43
1:A:97:TYR:CE1	1:A:214:GLN:NE2[3_746]	1.83	0.37
1:A:213:GLY:CA	1:A:247:TRP:CD1[3_756]	1.83	0.37
1:A:96:PRO:CA	5:A:412:HOH:O[3_746]	1.87	0.33



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Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1 1 22 77 0 00	4 4 242 4 627 627 627		1 ( )
1:A:96:PRO:CG	1:A:212:ASN:CB[3_746]	1.90	0.30
1:A:95:HIS:C	5:A:412:HOH:O[3_746]	1.92	0.28
1:A:97:TYR:CD2	1:A:214:GLN:OE1[3_746]	2.03	0.17
1:A:97:TYR:CZ	1:A:214:GLN:CD[3_746]	2.11	0.09
1:A:97:TYR:CE1	1:A:214:GLN:OE1[3_746]	2.13	0.07
1:A:97:TYR:OH	1:A:128:VAL:CG1[3_746]	2.14	0.06

#### 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	$238/240 \ (99\%)$	230 (97%)	8 (3%)	0	100 100	

There are no Ramachandran outliers to report.

#### 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	198/198 (100%)	191 (96%)	7 (4%)	36 38

All (7) residues with a non-rotameric sidechain are listed below:

$\mathbf{Mol}$	Chain	$\operatorname{Res}$	Type
1	A	36	ARG
1	A	51	ARG



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Mol	Chain	Res	Type
1	A	53	ASN
1	A	69	ARG
1	A	99	ASN
1	A	103	VAL
1	A	210	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	${f Res}$	Type
1	A	53	ASN
1	A	90	GLN
1	A	99	ASN
1	A	116	GLN
1	A	249	ASN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

#### 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

#### 5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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).



Mo	l Type	Chain	Chain Res L		Bond lengths			Bond angles		
IVIC	Type	Chain	nes	Link	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	0Z4	A	256	-	33,33,33	0.87	2 (6%)	45,45,45	1.82	9 (20%)
4	SO4	A	290	1	4,4,4	0.59	0	6,6,6	0.23	0

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	0Z4	A	256	_	-	14/39/39/39	0/1/1/1

#### All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}( ext{\AA})$
2	A	256	0Z4	C11-N11	-3.22	1.35	1.41
2	A	256	0Z4	C2-C1	2.15	1.58	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\mathbf{Ideal}(^o)$
2	A	256	0Z4	C3-CA1-N1	-5.92	95.03	111.16
2	A	256	0Z4	C-CA-N	-3.98	100.31	111.16
2	A	256	0Z4	CD2-CG1-CD1	-3.37	94.98	110.51
2	A	256	0Z4	CA1-C3-N11	-2.98	106.20	115.10
2	A	256	0Z4	O-C1-C2	2.80	123.76	118.31
2	A	256	0Z4	C3'-C1'-C2'	2.79	116.83	110.31
2	A	256	0Z4	CB1-CA1-C3	2.46	116.43	110.57
2	A	256	0Z4	O2-C3-N11	2.36	128.99	123.93
2	A	256	0Z4	CG1-CB1-CA1	2.06	121.11	115.43

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	256	0Z4	N-CA-CB-CG
2	A	256	0Z4	C-CA-CB-CG
2	A	256	0Z4	CA1-CB1-CG1-CD1
2	A	256	0Z4	O2-C3-N11-C11
2	A	256	0Z4	CA1-CB1-CG1-CD2
2	A	256	0Z4	CA1-C3-N11-C11
2	A	256	0Z4	O2-C3-CA1-N1



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Mol	Chain	Res	Type	Atoms
2	A	256	0Z4	N-C1-C2-F2
2	A	256	0Z4	O-C1-C2-F2
2	A	256	0Z4	N11-C3-CA1-N1
2	A	256	0Z4	N-C1-C2-F3
2	A	256	0Z4	O1-C-CA-CB
2	A	256	0Z4	N-C1-C2-F1
2	A	256	0Z4	N1-C-CA-CB

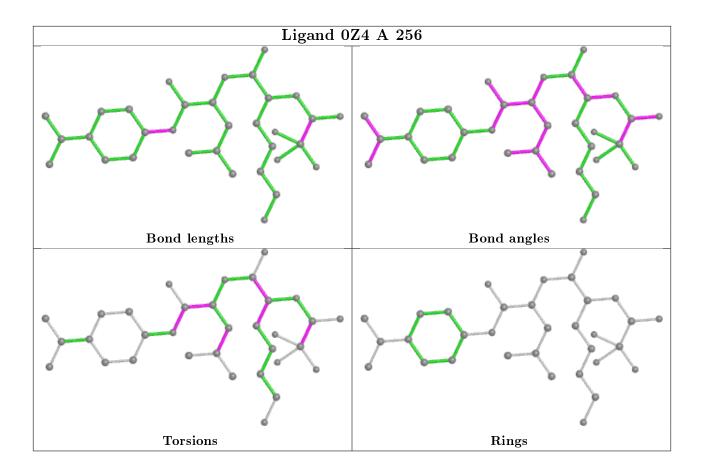
There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	256	0Z4	11	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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 (i)

#### 6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

#### 6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

#### 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

#### 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

