Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:54 PM GMT

PDB ID	:	1D3D
Title	:	CRYSTAL STRUCTURE OF HUMAN ALPHA THROMBIN IN COMPLEX WITH BENZOTHIOPHENE INHIBITOR 4
Authors	:	Chirgadze, N.Y.
Deposited on	:	1999-09-29
Resolution	:	2.04 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

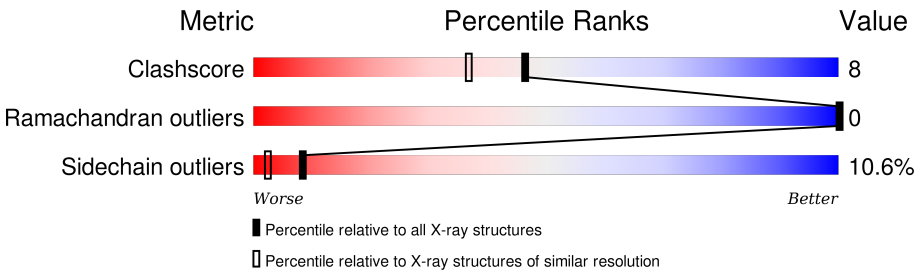
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.04 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	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)

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. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	28	71% 29%
2	B	257	79% 16% • •
3	H	12	67% 8% 25%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 2537 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 ALPHA-THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	28	231	145	37	48	1	0	0	0

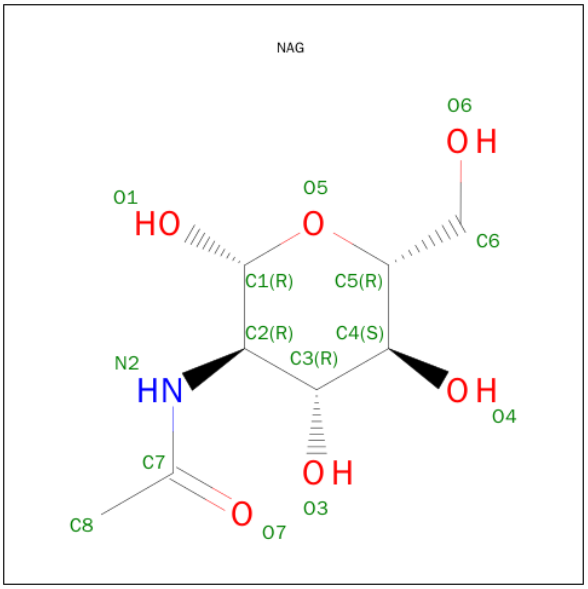
- Molecule 2 is a protein called ALPHA-THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	250	2025	1292	358	361	14	3	0	0

- Molecule 3 is a protein called HIRUGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	12	108	66	13	28	1	0	0	0

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

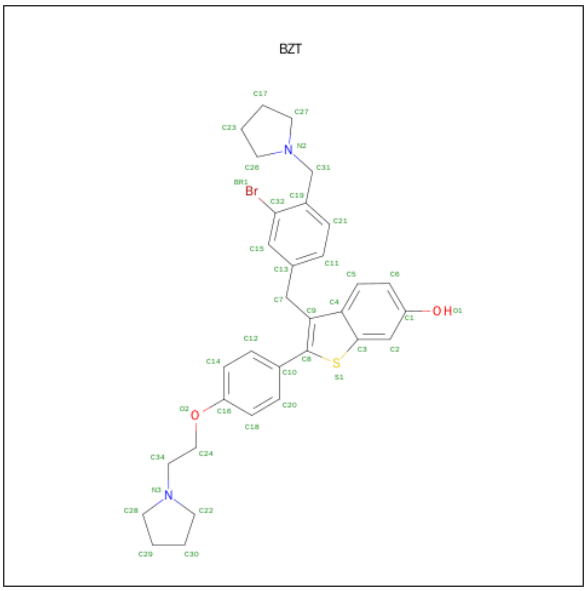


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	B	1	14	8	1	5	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
5	B	2	2	2	0	0

- Molecule 6 is 3-(3-BROMO-4-PYRROLIDIN-1-YLMETHYL-BENZYL)-2-[4-PYRROLIDIN-1-YL-ETHOXY)-PHENYL]-BENZO[B]THIOPHEN-6-OL (three-letter code: BZT) (formula: $C_{32}H_{35}BrN_2O_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	Br	C	N	O	S		
6	B	1	38	1	32	2	2	1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	12	12	12	0	0
7	B	107	Total	O	0	0
			107	107		

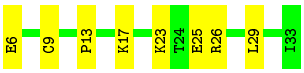
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

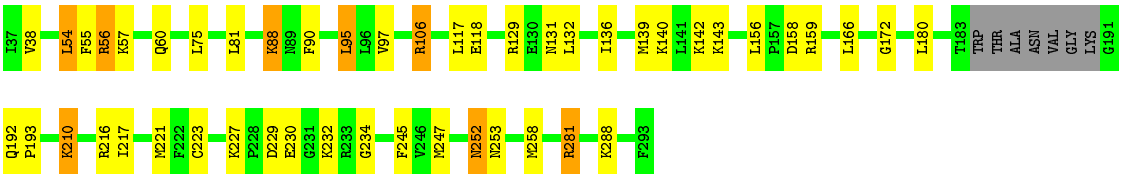
- Molecule 1: ALPHA-THROMBIN

Chain A:



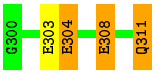
- Molecule 2: ALPHA-THROMBIN

Chain B:



- Molecule 3: HIRUGEN

Chain H:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	71.11Å 71.89Å 73.32Å 90.00° 100.60° 90.00°	Depositor
Resolution (Å)	20.00 – 2.04	Depositor
% Data completeness (in resolution range)	87.9 (20.00-2.04)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 98.0	Depositor
R, R_{free}	0.175 , 0.223	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2537	wwPDB-VP
Average B, all atoms (Å^2)	26.0	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: NA, BZT, NAG, TYS

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	0.41	0/233	0.66	0/310
2	B	0.39	0/2077	0.64	0/2806
3	H	0.43	0/92	0.47	0/120
All	All	0.40	0/2402	0.64	0/3236

There are no bond length outliers.

There are no bond angle outliers.

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)	H(added)	Clashes	Symm-Clashes
1	A	231	0	228	3	0
2	B	2025	0	2000	30	0
3	H	108	0	85	4	0
4	B	14	0	13	0	0
5	B	2	0	0	0	0
6	B	38	0	34	0	0
7	A	12	0	0	0	0
7	B	107	0	0	2	0
All	All	2537	0	2360	36	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 8.

All (36) 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)
2:B:281:ARG:HH11	2:B:281:ARG:HG3	1.48	0.78
2:B:106:ARG:HG2	3:H:303:GLU:OE1	1.87	0.73
2:B:118:GLU:OE2	2:B:140:LYS:HD3	1.97	0.65
2:B:129:ARG:HG3	7:B:593:HOH:O	1.98	0.64
2:B:180:LEU:HD21	2:B:193:PRO:HB3	1.80	0.62
2:B:281:ARG:HH11	2:B:281:ARG:CG	2.15	0.60
2:B:88:LYS:HD2	2:B:90:PHE:CE2	2.38	0.59
3:H:311:GLN:OXT	3:H:311:GLN:HG2	2.03	0.59
3:H:308:GLU:H	3:H:308:GLU:CD	2.06	0.58
2:B:56:ARG:O	2:B:60:GLN:HA	2.05	0.57
2:B:95:LEU:HD22	2:B:95:LEU:N	2.23	0.54
2:B:227:LYS:HB2	2:B:230:GLU:HG3	1.89	0.54
1:A:25:GLU:O	1:A:29:LEU:HD23	2.09	0.51
2:B:172:GLY:HA3	2:B:245:PHE:CZ	2.46	0.51
2:B:95:LEU:HD22	2:B:95:LEU:H	1.76	0.51
2:B:252:ASN:C	2:B:252:ASN:HD22	2.14	0.50
2:B:88:LYS:HD2	2:B:90:PHE:HE2	1.77	0.50
1:A:6:GLU:HB2	1:A:9:CYS:HB3	1.96	0.47
2:B:281:ARG:NH1	2:B:281:ARG:CG	2.74	0.47
2:B:55:PHE:CZ	2:B:60:GLN:HB3	2.51	0.46
1:A:13:PRO:HA	1:A:17:LYS:HG3	1.97	0.46
2:B:95:LEU:HD21	2:B:117:LEU:HD12	1.97	0.46
2:B:57:LYS:O	2:B:60:GLN:HG2	2.17	0.45
2:B:247:MET:SD	2:B:258:MET:HG3	2.57	0.45
2:B:210:LYS:HG3	2:B:217:ILE:HG12	1.99	0.44
2:B:281:ARG:NH1	2:B:281:ARG:HG3	2.24	0.44
3:H:304:GLU:HG3	3:H:304:GLU:H	1.49	0.43
2:B:38:VAL:O	2:B:234:GLY:HA2	2.19	0.43
2:B:95:LEU:CD2	2:B:117:LEU:HD12	2.50	0.42
2:B:216:ARG:HD2	7:B:589:HOH:O	2.19	0.42
2:B:54:LEU:HD21	2:B:139:MET:CE	2.50	0.41
2:B:131:ASN:O	2:B:132:LEU:HB2	2.21	0.41
2:B:252:ASN:C	2:B:252:ASN:ND2	2.74	0.41
2:B:166:LEU:HD23	2:B:166:LEU:HA	1.90	0.41
2:B:95:LEU:CD2	2:B:95:LEU:N	2.84	0.40
2:B:75:LEU:HD11	2:B:136:ILE:HD11	2.03	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	26/28 (93%)	25 (96%)	1 (4%)	0	100	100
2	B	246/257 (96%)	240 (98%)	6 (2%)	0	100	100
3	H	9/12 (75%)	9 (100%)	0	0	100	100
All	All	281/297 (95%)	274 (98%)	7 (2%)	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	26/26 (100%)	24 (92%)	2 (8%)	16	7
2	B	219/224 (98%)	197 (90%)	22 (10%)	9	3
3	H	10/10 (100%)	7 (70%)	3 (30%)	0	0
All	All	255/260 (98%)	228 (89%)	27 (11%)	8	2

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	26	ARG
2	B	54	LEU
2	B	56	ARG
2	B	81	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	88	LYS
2	B	95	LEU
2	B	97	VAL
2	B	106	ARG
2	B	142	LYS
2	B	143	LYS
2	B	156	LEU
2	B	158	ASP
2	B	159	ARG
2	B	192	GLN
2	B	210	LYS
2	B	221	MET
2	B	223	CYS
2	B	229	ASP
2	B	232	LYS
2	B	252	ASN
2	B	253	ASN
2	B	281	ARG
2	B	288	LYS
3	H	304	GLU
3	H	308	GLU
3	H	311	GLN

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

Mol	Chain	Res	Type
2	B	60	GLN
2	B	192	GLN
2	B	252	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)

1 non-standard protein/DNA/RNA residue 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	$\#\|Z\| > 2$
3	TYS	H	309	3	15,16,17	4.67	10 (66%)	16,22,24	0.98	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
3	TYS	H	309	3	-	0/9/11/13	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	309	TYS	OH-S	-6.23	1.52	1.63
3	H	309	TYS	OH-CZ	-3.30	1.37	1.42
3	H	309	TYS	O1-S	2.49	1.54	1.45
3	H	309	TYS	O2-S	2.73	1.55	1.45
3	H	309	TYS	CD1-CG	5.76	1.51	1.38
3	H	309	TYS	CE2-CZ	6.01	1.50	1.38
3	H	309	TYS	CD2-CG	6.26	1.52	1.38
3	H	309	TYS	CE1-CZ	6.65	1.52	1.38
3	H	309	TYS	CE2-CD2	7.28	1.51	1.38
3	H	309	TYS	CE1-CD1	7.45	1.52	1.38

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	BZT	B	400	-	39,43,43	2.35	17 (43%)	47,60,60	2.59	18 (38%)
4	NAG	B	500	2	14,14,15	0.76	0	15,19,21	1.21	1 (6%)

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
6	BZT	B	400	-	-	0/18/32/32	0/6/6/6
4	NAG	B	500	2	-	0/6/23/26	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	400	BZT	BR1-C32	-3.18	1.81	1.89
6	B	400	BZT	C7-C9	-2.97	1.48	1.52
6	B	400	BZT	C11-C13	2.05	1.43	1.38
6	B	400	BZT	C21-C19	2.06	1.43	1.39
6	B	400	BZT	C20-C10	2.16	1.43	1.39
6	B	400	BZT	C15-C13	2.31	1.43	1.39
6	B	400	BZT	O2-C16	2.61	1.43	1.37
6	B	400	BZT	C20-C18	2.95	1.44	1.38
6	B	400	BZT	C10-C8	3.08	1.51	1.48
6	B	400	BZT	C7-C13	3.27	1.63	1.52
6	B	400	BZT	C26-N2	3.29	1.53	1.47
6	B	400	BZT	C15-C32	3.30	1.45	1.38
6	B	400	BZT	C2-C3	3.40	1.43	1.37
6	B	400	BZT	C12-C10	3.69	1.47	1.39
6	B	400	BZT	C18-C16	4.08	1.46	1.38
6	B	400	BZT	C5-C6	4.33	1.45	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	400	BZT	C2-C1	4.56	1.46	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	400	BZT	C27-N2-C26	-7.68	96.22	104.08
6	B	400	BZT	C7-C9-C8	-6.52	116.75	127.34
6	B	400	BZT	C29-C28-N3	-4.18	99.16	103.91
6	B	400	BZT	BR1-C32-C15	-3.48	112.30	118.42
6	B	400	BZT	C30-C22-N3	-3.40	100.05	103.91
6	B	400	BZT	C28-N3-C22	-3.10	100.92	104.08
6	B	400	BZT	C17-C27-N2	-2.83	100.70	103.91
4	B	500	NAG	C4-C3-C2	-2.69	107.05	111.23
6	B	400	BZT	C17-C23-C26	-2.61	97.67	105.29
6	B	400	BZT	C18-C20-C10	-2.36	117.69	121.14
6	B	400	BZT	C6-C1-C2	-2.26	117.03	120.34
6	B	400	BZT	C11-C21-C19	2.34	124.66	121.41
6	B	400	BZT	C1-C2-C3	2.61	123.11	120.36
6	B	400	BZT	C9-C7-C13	2.72	119.88	113.64
6	B	400	BZT	C20-C18-C16	2.75	123.20	119.74
6	B	400	BZT	O2-C24-C34	3.25	115.17	107.67
6	B	400	BZT	C31-N2-C26	3.52	118.47	113.10
6	B	400	BZT	BR1-C32-C19	4.10	125.77	120.32
6	B	400	BZT	C31-N2-C27	6.64	123.24	113.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.