wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 07:01 PM GMT

PDB ID	:	1DLP
Title	:	STRUCTURAL CHARACTERIZATION OF THE NATIVE FETUIN-BINDING PROTEIN SCILLA CAMPANULATA AGGLUTININ (SCAFET): A NOVEL TWO-DOMAIN LECTIN
Authors	:	Wright, L.M.; Reynolds, C.D.; Rizkallah, P.J.; Allen, A.K.; VanDamme, E.J.M.; Donovan, M.J.; Peumans, W.J.
Deposited on	:	1999-12-11
Resolution	:	3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

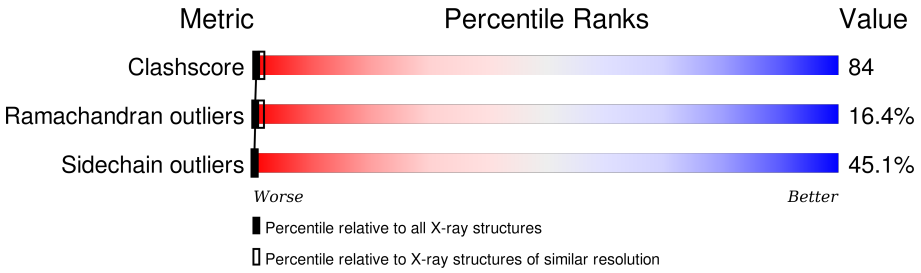
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.30 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	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)

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	236	13% 35% 51%
1	B	236	11% 34% 48% 6%
1	C	236	17% 32% 48%
1	D	236	11% 35% 49% 6%
1	E	236	14% 39% 43%
1	F	236	14% 37% 40% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10431 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 LECTIN SCAFET PRECURSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	18	0	0
			1778	1102	322	347	7			
1	B	221	Total	C	N	O	S	21	0	0
			1694	1053	305	329	7			
1	C	234	Total	C	N	O	S	25	0	0
			1772	1097	323	345	7			
1	D	223	Total	C	N	O	S	28	0	0
			1702	1057	307	331	7			
1	E	231	Total	C	N	O	S	17	0	0
			1759	1093	318	341	7			
1	F	216	Total	C	N	O	S	40	0	0
			1659	1034	298	320	7			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	19	Total	O	0	0
			19	19		
2	B	15	Total	O	0	0
			15	15		
2	C	6	Total	O	0	0
			6	6		
2	D	8	Total	O	0	0
			8	8		
2	E	8	Total	O	0	0
			8	8		
2	F	11	Total	O	0	0
			11	11		

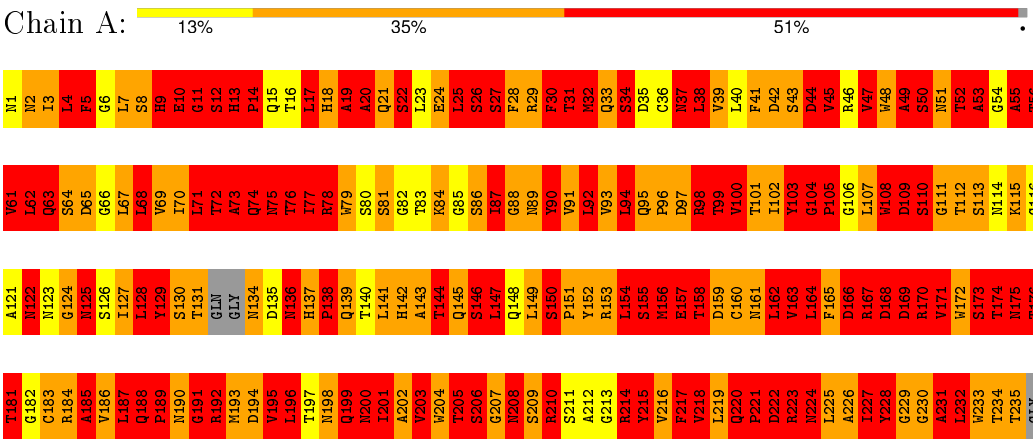
3 Residue-property plots (i)

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.

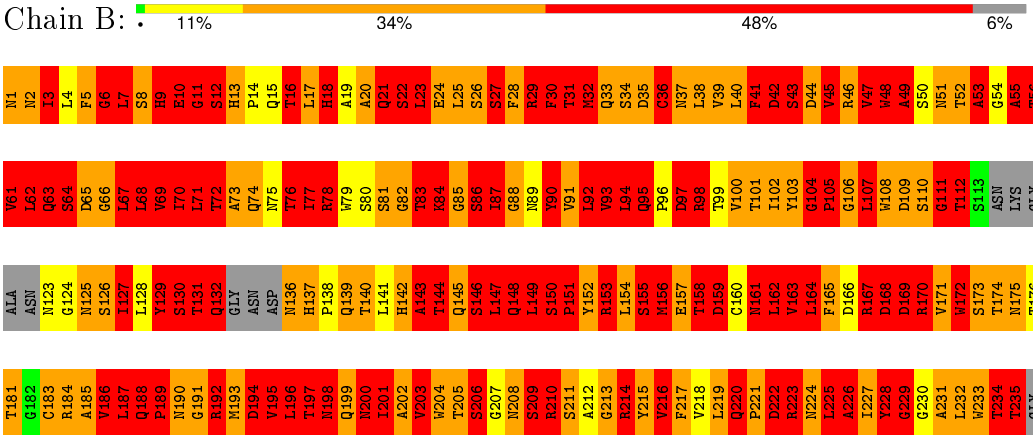
- Molecule 1: LECTIN SCAFET PRECURSOR

Chain A:



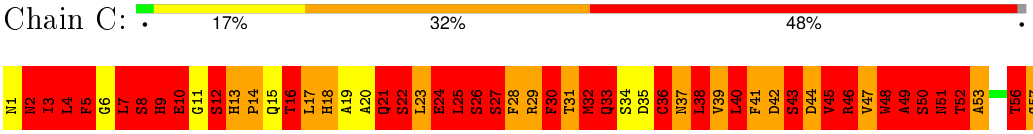
- Molecule 1: LECTIN SCAFET PRECURSOR

Chain B:



- Molecule 1: LECTIN SCAFET PRECURSOR

Chain C:



L62 Q63 S64 D65 G66 L67 L68 V69 I70 L71 T72 A73 Q74 N75 T76 I77 R78 W79 S80 S81 G82 T83 K84 G85 S86 I87 G88 N89 Y90 V91 L92 V93 L94 Q95 P96 D97 R98 T99 V100 T101 I102 Y103 G104 P105 G106 L107 W108 D109 S110 G111 T112 S113 N114 K115 G116 S117 V118 V119 V120 A121

N122 N123 G124 N125 S126 I127 L128 Y129 S130 T131 Q132 G133 ASN ASP N136 H137 P138 Q139 T140 L141 H142 A143 T144 Q145 S146 L147 Q148 L149 S150 P151 Y152 R153 L154 S155 M156 E157 T158 D159 C160 N161 L162 V163 L164 F165 D166 R167 D168 D169 R170 V171 W172 S173 T174 N175 T176 A177 G178 K179 G180 T181

G182 C183 R184 A185 V186 L187 Q188 P189 N190 G191 R192 M193 D194 V195 L196 T197 N198 Q199 N200 I201 A202 V203 W204 T205 S206 G207 N208 S209 R210 S211 A212 G213 R214 Y215 V216 F217 V218 L219 Q220 P221 D222 R223 N224 L225 A226 I227 Y228 G229 G230 A231 L232 W233 T234 T235 G236

- Molecule 1: LECTIN SCAFET PRECURSOR

Chain D: 11% 35% 49% 6%

N1 N2 I3 L4 F5 G6 L7 S8 H9 E10 G11 S12 H13 P14 Q15 T16 L17 H18 A19 A20 Q21 S22 L23 E24 L25 S26 S27 F28 R29 F30 T31 M32 Q33 S34 D35 C36 N37 L38 V39 L40 F41 D42 S43 D44 V45 R46 V47 W48 A49 S50 N51 T52 A53 G54 A55 T56 G57 C58 R59 A60

V61 L62 Q63 S64 D65 G66 L67 L68 V69 I70 L71 T72 A73 Q74 N75 T76 I77 R78 W79 S80 S81 G82 T83 K84 G85 S86 I87 G88 N89 Y90 V91 L92 V93 L94 Q95 P96 D97 R98 T99 V100 T101 I102 Y103 G104 P105 G106 L107 W108 D109 S110 G111 T112 S113 N114 LYS GLY SER VAL VAL

ALA ASN N123 G124 N125 S126 I127 L128 Y129 S130 T131 GLN GLY ASN ASP N136 H137 P138 Q139 T140 L141 H142 A143 T144 Q145 S146 L147 Q148 L149 S150 P151 Y152 R153 L154 S155 M156 E157 T158 D159 C160 N161 L162 V163 L164 F165 D166 R167 D168 D169 R170 V171 W172 S173 T174 N175 T176 A177 G178 K179 G180

T181 G182 C183 R184 A185 V186 L187 Q188 P189 N190 G191 R192 M193 D194 V195 L196 T197 N198 Q199 N200 I201 A202 V203 W204 T205 S206 G207 N208 S209 R210 S211 A212 G213 R214 Y215 V216 F217 V218 L219 Q220 P221 D222 R223 N224 L225 A226 I227 Y228 G229 G230 A231 L232 W233 T234 T235 GLY

- Molecule 1: LECTIN SCAFET PRECURSOR

Chain E: • 14% 39% 43% •

N1 N2 I3 L4 F5 G6 L7 S8 H9 E10 G11 S12 H13 P14 Q15 T16 L17 H18 A19 A20 Q21 S22 L23 E24 L25 S26 S27 F28 R29 F30 T31 M32 Q33 S34 D35 C36 N37 L38 V39 L40 F41 D42 S43 D44 V45 R46 V47 W48 A49 S50 N51 T52 A53 G54 A55 T56 G57 C58 R59 A60

V61 L62 Q63 S64 D65 G66 L67 L68 V69 I70 L71 T72 A73 Q74 N75 T76 I77 R78 W79 S80 S81 G82 T83 K84 G85 S86 I87 G88 N89 Y90 V91 L92 V93 L94 Q95 P96 D97 R98 T99 V100 T101 I102 Y103 G104 P105 G106 L107 W108 D109 S110 G111 T112 S113 N114 K115 G116 S117 V118 V119 V120

A121 N122 N123 G124 N125 S126 I127 L128 Y129 S130 T131 GLN GLY ASN ASP N136 H137 P138 Q139 T140 L141 H142 A143 T144 Q145 S146 L147 Q148 L149 S150 P151 Y152 R153 L154 S155 M156 E157 T158 D159 C160 N161 L162 V163 L164 F165 D166 R167 D168 D169 R170 V171 W172 S173 T174 N175 T176 A177 G178 K179 G180

T181 G182 C183 R184 A185 V186 L187 Q188 P189 N190 G191 R192 M193 D194 V195 L196 T197 N198 Q199 N200 I201 A202 V203 W204 T205 S206 G207 N208 S209 R210 S211 A212 G213 R214 Y215 V216 F217 V218 L219 Q220 P221 D222 R223 N224 L225 A226 I227 Y228 G229 G230 A231 L232 W233 T234 T235 GLY

- Molecule 1: LECTIN SCAFET PRECURSOR

Chain F: • 14% 37% 40% 8%

N1 N2 I3 L4 F5 G6 L7 S8 H9 E10 G11 S12 H13 P14 Q15 T16 L17 H18 A19 A20 Q21 S22 L23 E24 L25 S26 S27 F28 R29 F30 T31 M32 Q33 S34 D35 C36 N37 L38 V39 L40 F41 D42 S43 D44 V45 R46 V47 W48 A49 S50 N51 T52 A53 G54 A55 T56 G57 C58 R59 A60

V61 L62 Q63 S64 D65 G66 L67 L68 V69 I70 L71 T72 A73 Q74 N75 T76 I77 R78 W79 S80 S81 G82 T83 K84 G85 S86 I87 G88 N89 Y90 V91 L92 V93 L94 Q95 P96 D97 R98 T99 V100 T101 I102 Y103 G104 P105 G106 L107 W108 D109 S110 G111 THR SER ASN LYS GLY SER VAL VAL


ALA
ASN
ASN
G124
N125
S126
I127
L128
Y129
S130
T131
GLN
GLY
ASN
ASP
N136
H137
P138
Q139
T140
L141
H142
A143
T144
Q145
S146
L147
Q148
L149
S150
P151
Y152
R153
L154
S155
M156
E157
T158
D159
C160
N161
L162
V163
L164
F165
D166
R167
D168
D169
R170
V171
W172
S173
T174
N175
T176
ALA
GLY
LYS
G180


T181
G182
C183
R184
A185
V186
L187
Q188
P189
N190
G191
R192
M193
D194
V195
L196
T197
N198
Q199
N200
I201
A202
V203
W204
T205
S206
G207
M208
S209
R210
S211
A212
G213
R214
Y215
V216
F217
V218
L219
Q220
P221
D222
R223
N224
L225
A226
I227
Y228
G229
G230
A231
L232
W233
T234
T235
GLY

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	277.94Å 164.10Å 53.60Å 90.00° 95.38° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30	Depositor
% Data completeness (in resolution range)	95.3 (20.00-3.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.189 , 0.293	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10431	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	2.62	91/1812 (5.0%)	6.89	912/2470 (36.9%)
1	B	2.44	80/1726 (4.6%)	6.84	897/2351 (38.2%)
1	C	2.34	58/1805 (3.2%)	6.48	838/2459 (34.1%)
1	D	3.14	88/1735 (5.1%)	7.13	928/2365 (39.2%)
1	E	2.06	35/1793 (2.0%)	5.99	765/2444 (31.3%)
1	F	2.14	38/1691 (2.2%)	6.60	810/2303 (35.2%)
All	All	2.48	390/10562 (3.7%)	6.66	5150/14392 (35.8%)

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	2	60
1	B	2	73
1	C	0	66
1	D	0	51
1	E	0	39
1	F	2	53
All	All	6	342

The worst 5 of 390 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1	ASN	CG-ND2	50.13	2.58	1.32
1	D	78	ARG	CG-CD	46.82	2.69	1.51
1	A	44	ASP	CB-CG	-34.10	0.80	1.51
1	C	168	ASP	CG-OD1	30.06	1.94	1.25
1	D	167	ARG	CD-NE	-29.28	0.96	1.46

The worst 5 of 5150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	214	ARG	NE-CZ-NH2	59.84	150.22	120.30
1	E	59	ARG	NE-CZ-NH2	-55.14	92.73	120.30
1	B	184	ARG	NE-CZ-NH2	-53.22	93.69	120.30
1	F	223	ARG	NE-CZ-NH2	-49.78	95.41	120.30
1	A	184	ARG	NE-CZ-NH1	48.82	144.71	120.30

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	9	HIS	CA
1	A	87	ILE	CA
1	B	60	ALA	CA
1	B	168	ASP	CA
1	F	60	ALA	CA

5 of 342 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	HIS	Mainchain
1	A	19	ALA	Mainchain
1	A	2	ASN	Peptide
1	A	25	LEU	Mainchain
1	A	5	PHE	Mainchain

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	1778	0	1700	282	0
1	B	1694	0	1600	265	0
1	C	1772	0	1695	270	0
1	D	1702	0	1613	321	0
1	E	1759	0	1684	310	0
1	F	1659	0	1579	305	0
2	A	19	0	0	1	0
2	B	15	0	0	0	0
2	C	6	0	0	0	0
2	D	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	8	0	0	0	0
2	F	11	0	0	0	0
All	All	10431	0	9871	1677	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 84.

The worst 5 of 1677 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:D:77:ILE:CD1	1:D:77:ILE:CG1	1.80	1.57
1:E:131:THR:CA	1:E:131:THR:C	1.75	1.50
1:E:136:ASN:CA	1:E:136:ASN:CB	1.88	1.49
1:A:131:THR:CB	1:A:131:THR:OG1	1.64	1.46
1:D:64:SER:OG	1:D:64:SER:CB	1.67	1.43

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	229/236 (97%)	158 (69%)	41 (18%)	30 (13%)	0	2
1	B	213/236 (90%)	132 (62%)	42 (20%)	39 (18%)	0	1
1	C	230/236 (98%)	150 (65%)	42 (18%)	38 (16%)	0	1
1	D	217/236 (92%)	148 (68%)	30 (14%)	39 (18%)	0	1
1	E	227/236 (96%)	150 (66%)	39 (17%)	38 (17%)	0	1
1	F	208/236 (88%)	138 (66%)	37 (18%)	33 (16%)	0	1
All	All	1324/1416 (94%)	876 (66%)	231 (17%)	217 (16%)	0	1

5 of 217 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	A	11	GLY
1	A	14	PRO
1	A	19	ALA
1	A	20	ALA

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	197/198 (100%)	99 (50%)	98 (50%)	0	0
1	B	187/198 (94%)	96 (51%)	91 (49%)	0	0
1	C	195/198 (98%)	111 (57%)	84 (43%)	0	0
1	D	187/198 (94%)	101 (54%)	86 (46%)	0	0
1	E	194/198 (98%)	112 (58%)	82 (42%)	0	0
1	F	183/198 (92%)	108 (59%)	75 (41%)	0	0
All	All	1143/1188 (96%)	627 (55%)	516 (45%)	0	0

5 of 516 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	137	HIS
1	D	48	TRP
1	F	127	ILE
1	C	150	SER
1	C	203	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	125	ASN
1	D	18	HIS

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Mol	Chain	Res	Type
1	F	161	ASN
1	C	136	ASN
1	C	161	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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