



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:49 PM GMT

PDB ID : 3S6P
Title : Crystal Structure of Helicoverpa Armigera Stunt Virus
Authors : Speir, J.A.; Chen, Z.; Taylor, D.J.; Johnson, J.E.
Deposited on : 2011-05-25
Resolution : 2.50 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : **FAILED**
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

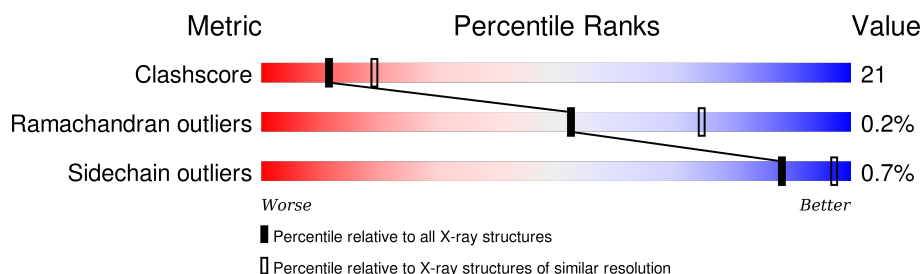
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)


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 $\leq 5\%$. 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 failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	575	
1	B	575	
1	C	575	
1	D	575	
2	E	72	
2	F	72	
2	G	72	

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Mol	Chain	Length	Quality of chain
2	H	72	 A horizontal bar chart showing the quality of chain H. The bar is divided into three segments: green (54%), yellow (33%), and grey (13%).

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 19383 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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	S	0	4	0
			4145	2629	695	809	12			
1	B	530	Total	C	N	O	S	0	3	0
			4143	2628	694	809	12			
1	C	536	Total	C	N	O	S	0	2	0
			4182	2652	704	814	12			
1	D	532	Total	C	N	O	S	0	6	0
			4177	2652	701	811	13			

- Molecule 2 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	33	Total	C	N	O	S	0	0	0
			227	143	36	47	1			
2	F	24	Total	C	N	O	S	0	0	0
			164	103	26	34	1			
2	G	72	Total	C	N	O	S	0	5	0
			547	339	112	93	3			
2	H	63	Total	C	N	O	S	0	5	0
			485	300	99	83	3			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0

- Molecule 5 is water.

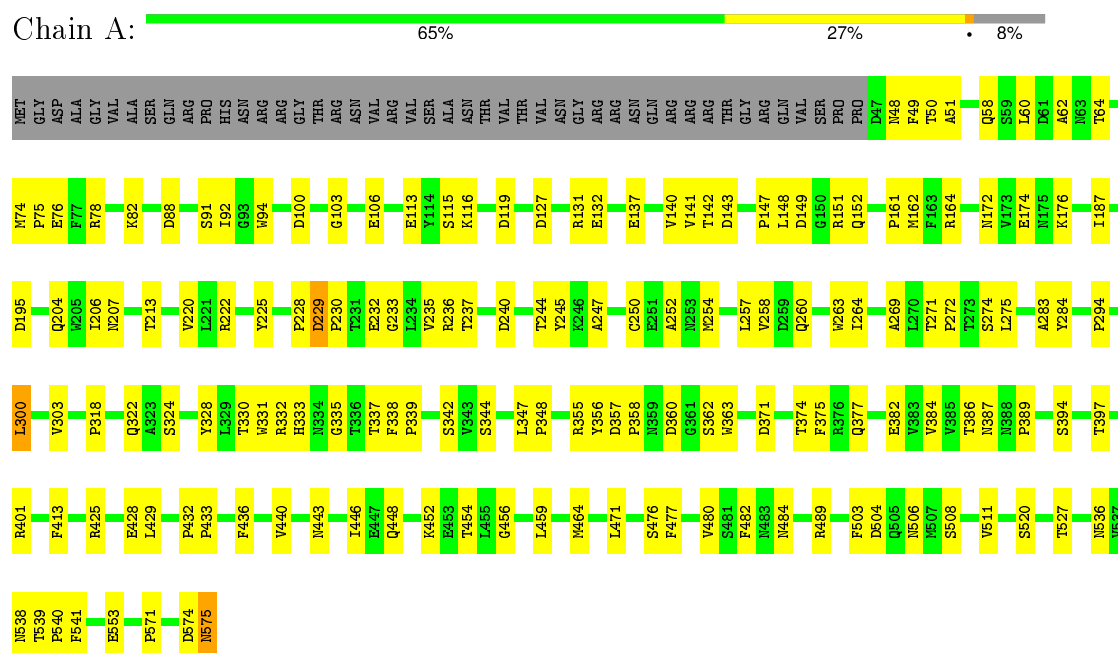
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	330	Total O 330 330	0	0
5	E	7	Total O 7 7	0	0
5	B	313	Total O 313 313	0	0
5	F	4	Total O 4 4	0	0
5	C	290	Total O 290 290	0	0
5	G	43	Total O 43 43	0	0
5	D	287	Total O 287 287	0	0
5	H	35	Total O 35 35	0	0

3 Residue-property plots [i](#)

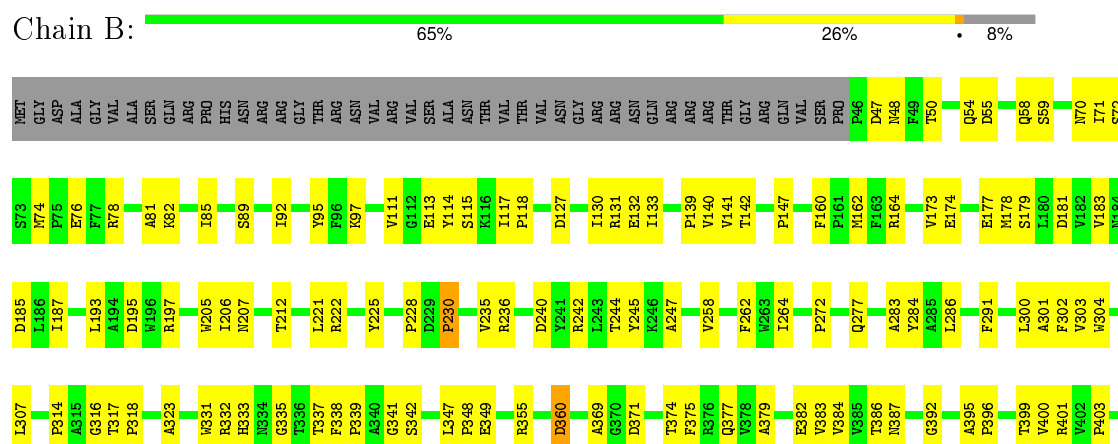
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

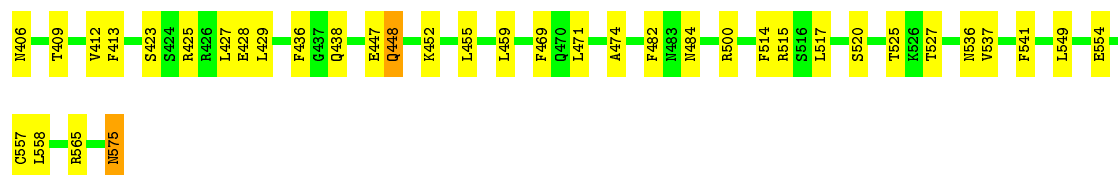
Note EDS failed to run properly.

- Molecule 1: Capsid protein



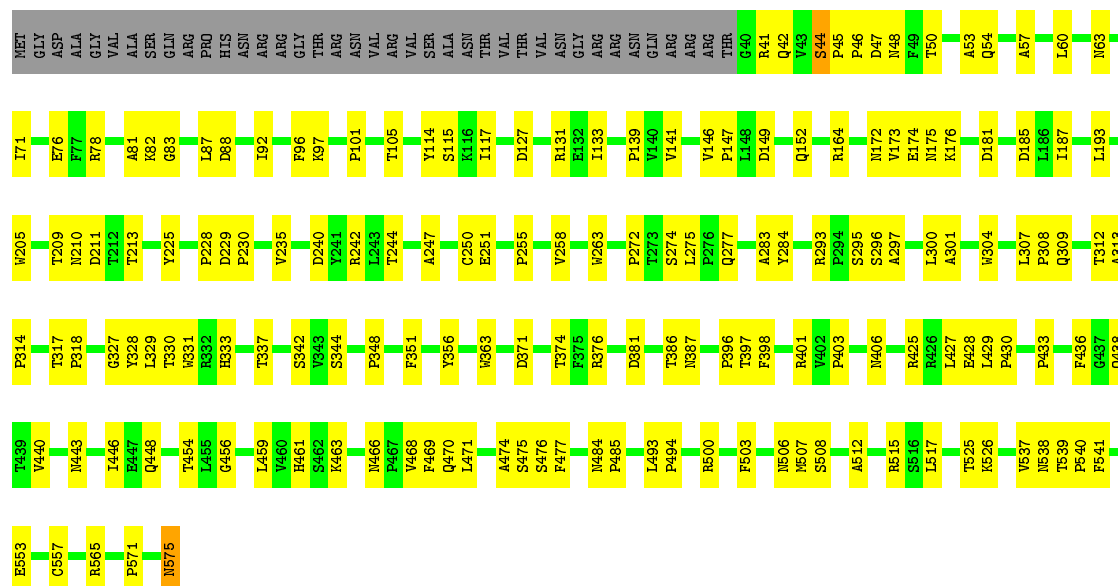
- Molecule 1: Capsid protein





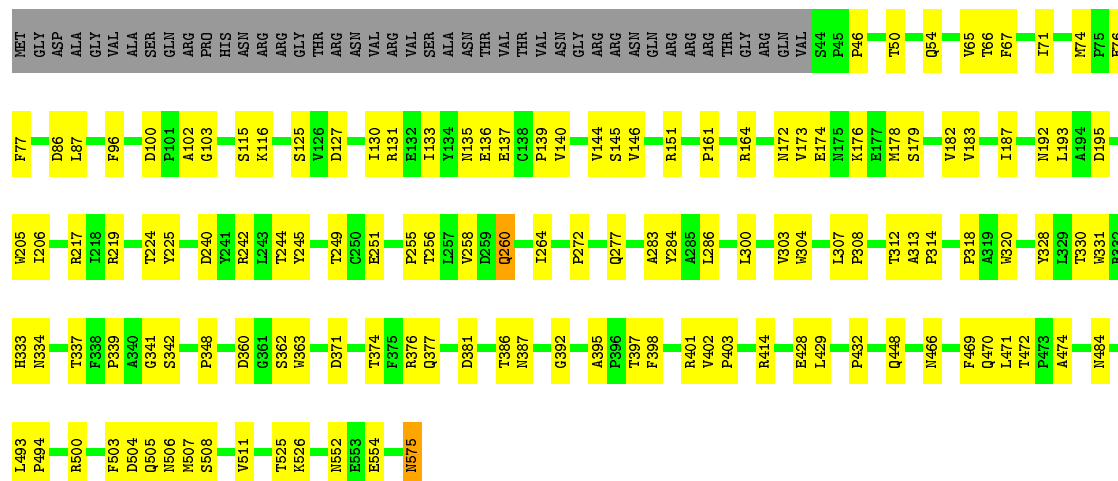
• Molecule 1: Capsid protein

Chain C: 65% 28% 7%



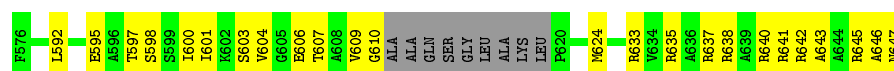
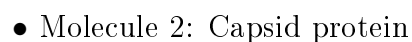
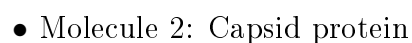
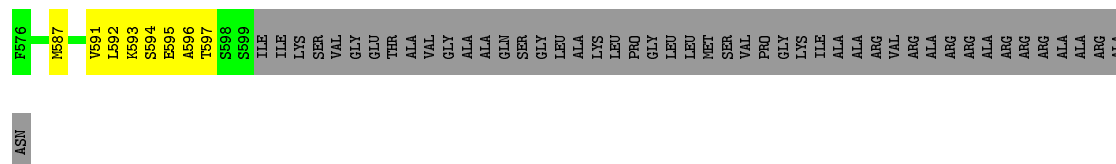
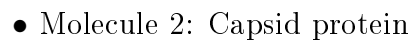
• Molecule 1: Capsid protein

Chain D: 70% 23% 7%



• Molecule 2: Capsid protein

Chain E: 32% 14% 54%



4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	404.12Å 405.57Å 406.04Å 119.20° 114.44° 94.79°	Depositor
Resolution (Å)	40.00 – 2.50	Depositor
% Data completeness (in resolution range)	27.3 (40.00-2.50)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.237 , (Not available)	Depositor
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.132	Xtriage
Estimated twinning fraction	0.002 for k,h,-h-k-l 0.002 for l,-h-k-l,h 0.002 for -h-k-l,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 1807472 reflections	Xtriage
Total number of atoms	19383	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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: CA, CL

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	0.56	0/4270	0.74	0/5846
1	B	0.55	0/4266	0.73	0/5842
1	C	0.55	0/4303	0.74	1/5892 (0.0%)
1	D	0.56	0/4311	0.74	0/5902
2	E	0.52	0/228	0.57	0/307
2	F	0.62	0/165	0.56	0/222
2	G	0.54	0/565	0.73	0/753
2	H	0.57	0/502	0.69	0/664
All	All	0.55	0/18610	0.73	1/25428 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	44	SER	C-N-CD	-5.05	109.49	120.60

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	4145	0	3962	172	0
1	B	4143	0	3957	176	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4182	0	4002	169	0
1	D	4177	0	4004	137	0
2	E	227	0	233	25	0
2	F	164	0	163	10	0
2	G	547	0	608	61	0
2	H	485	0	535	41	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	330	0	0	18	0
5	B	313	0	0	5	0
5	C	290	0	0	13	0
5	D	287	0	0	8	0
5	E	7	0	0	0	0
5	F	4	0	0	0	0
5	G	43	0	0	9	0
5	H	35	0	0	8	0
All	All	19383	0	17464	730	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 21.

The worst 5 of 730 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:B:181:ASP:CB	1:D:334:ASN:HD22	1.44	1.28
1:C:44:SER:OG	1:C:45:PRO:HA	1.36	1.23
1:A:575:ASN:C	1:A:575:ASN:HD22	1.46	1.15
2:G:593:LYS:HD3	2:G:601:ILE:HD13	1.25	1.13
1:B:575:ASN:C	1:B:575:ASN:HD22	1.49	1.12

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	531/575 (92%)	509 (96%)	21 (4%)	1 (0%)	52	75
1	B	531/575 (92%)	509 (96%)	21 (4%)	1 (0%)	52	75
1	C	536/575 (93%)	512 (96%)	23 (4%)	1 (0%)	52	75
1	D	536/575 (93%)	517 (96%)	19 (4%)	0	100	100
2	E	31/72 (43%)	31 (100%)	0	0	100	100
2	F	22/72 (31%)	22 (100%)	0	0	100	100
2	G	75/72 (104%)	71 (95%)	3 (4%)	1 (1%)	15	26
2	H	63/72 (88%)	62 (98%)	1 (2%)	0	100	100
All	All	2325/2588 (90%)	2233 (96%)	88 (4%)	4 (0%)	52	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	296	SER
2	G	609	VAL
1	A	229	ASP
1	B	230	PRO

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	449/483 (93%)	446 (99%)	3 (1%)	88	97
1	B	449/483 (93%)	446 (99%)	3 (1%)	88	97
1	C	453/483 (94%)	450 (99%)	3 (1%)	88	97
1	D	454/483 (94%)	452 (100%)	2 (0%)	93	98
2	E	24/49 (49%)	24 (100%)	0	100	100
2	F	17/49 (35%)	17 (100%)	0	100	100
2	G	54/49 (110%)	52 (96%)	2 (4%)	41	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	49/49 (100%)	48 (98%)	1 (2%)	63	86
All	All	1949/2128 (92%)	1935 (99%)	14 (1%)	88	97

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	149	ASP
1	C	229	ASP
1	D	260	GLN
1	B	575	ASN
2	G	624[B]	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	333	HIS
1	C	461	HIS
1	D	466	ASN
1	C	388	ASN
1	C	466	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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

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.

5.7 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 failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.