



# Full wwPDB X-ray Structure Validation Report

May 29, 2014 – 01:10 AM EDT

PDB ID : 4O46  
Title : 14-3-3-gamma in complex with influenza NS1 C-terminal tail phosphorylated at S228  
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Deposited on : 2013-12-18  
Resolution : 2.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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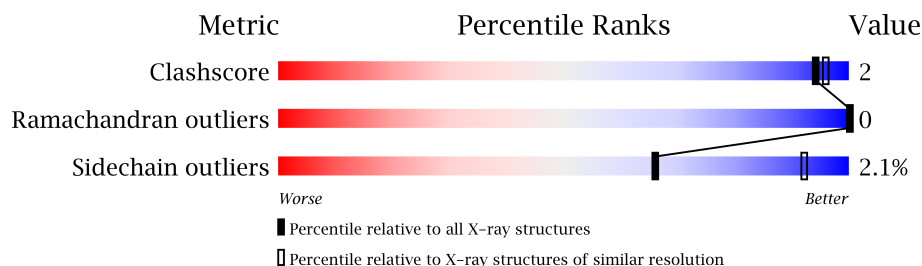
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : **FAILED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23161

# 1 Overall quality at a glance

The reported resolution of this entry is 2.90 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	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	256	
1	B	256	
1	C	256	
1	D	256	
1	E	256	
1	F	256	
2	G	15	
2	H	15	
2	I	15	
2	J	15	
2	K	15	
2	L	15	
3	M	24	
3	N	24	
3	O	24	
3	V	24	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10919 atoms, of which 0 are hydrogen and 0 are deuterium.

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 14-3-3 protein gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	0	1	0
			1811	1135	314	353	9			
1	B	234	Total	C	N	O	S	0	0	0
			1818	1142	306	361	9			
1	C	235	Total	C	N	O	S	0	1	0
			1804	1134	303	358	9			
1	D	235	Total	C	N	O	S	0	0	0
			1777	1116	304	347	10			
1	E	236	Total	C	N	O	S	0	0	0
			1814	1138	312	355	9			
1	F	206	Total	C	N	O	S	0	0	0
			1354	841	243	265	5			

- Molecule 2 is a protein called Nonstructural protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	6	Total	C	N	O	P	0	0	0
			42	24	7	10	1			
2	H	6	Total	C	N	O	P	0	0	0
			42	24	6	11	1			
2	I	6	Total	C	N	O	P	0	0	0
			44	25	7	11	1			
2	J	6	Total	C	N	O	P	0	0	0
			40	23	6	10	1			
2	K	6	Total	C	N	O	P	0	0	0
			41	24	6	10	1			
2	L	2	Total	C	N	O	P	0	0	0
			15	6	2	6	1			

- Molecule 3 is a protein called Unidentified polymer.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	20	Total	C	N	O	0	0	0
			100	60	20	20			
3	N	9	Total	C	N	O	0	0	0
			45	27	9	9			
3	O	10	Total	C	N	O	0	0	0
			50	30	10	10			
3	V	13	Total	C	N	O	0	0	0
			65	39	13	13			

- Molecule 4 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	9	Total	X	0	0
			9	9		
4	E	5	Total	X	0	0
			5	5		
4	B	18	Total	X	0	0
			18	18		
4	C	14	Total	X	0	0
			14	14		
4	A	10	Total	X	0	0
			10	10		
4	F	1	Total	X	0	0
			1	1		

### 3 Residue-property plots

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: 14-3-3 protein gamma

Chain A: 



- Molecule 1: 14-3-3 protein gamma

Chain B: 



- Molecule 1: 14-3-3 protein gamma

Chain C: 



- Molecule 1: 14-3-3 protein gamma

Chain D: 



- Molecule 1: 14-3-3 protein gamma

Chain E: 



- Molecule 1: 14-3-3 protein gamma

Chain F: 



S235	ASP
	GLN
	GLN
	ASP
	ASP
	ASP
	GLY
	GLY
	GLY
	ASN
	ASN
	SER
	LEU
	GLU
	HIS
	HIS
	HIS
	HIS

- Molecule 2: Nonstructural protein 1

Chain G: 

PRO	LYS	GLN
	LYS	ARG
	LYS	MET
	ALA	ARG
	T225	
	T225	
	V230	

- Molecule 2: Nonstructural protein 1

Chain H: 

PRO	LYS	GLN
	LYS	ARG
	LYS	MET
	ALA	ARG
	T225	
	A226	
	T225	
	V230	

- Molecule 2: Nonstructural protein 1

Chain I: 

PRO	LYS	GLN
	LYS	ARG
	LYS	MET
	ALA	ARG
	T225	
	T225	
	V230	

- Molecule 2: Nonstructural protein 1

Chain J: 

PRO	LYS	GLN
	LYS	ARG
	LYS	MET
	ALA	ARG
	T225	
	T225	
	V230	

- Molecule 2: Nonstructural protein 1

Chain K: 

PRO	LYS	GLN
	LYS	ARG
	LYS	MET
	ALA	ARG
	T225	
	T225	
	V230	

- Molecule 2: Nonstructural protein 1

Chain L: 

PRO	LYS	GLN
	LYS	ARG
	LYS	MET
	ALA	THR
	ALA	ARG
	S228	
	K229	
	VAL	

- Molecule 3: Unidentified polymer

Chain M: 

X6	X25
	UNK
	UNK
	UNK

- Molecule 3: Unidentified polymer

Chain N: 

X10	X18	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK
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- Molecule 3: Unidentified polymer

Chain O:

X10	X19	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK
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- Molecule 3: Unidentified polymer

Chain V:

X7	X19	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK
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## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.83Å 121.83Å 314.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.53 – 2.90	Depositor
% Data completeness (in resolution range)	100.0 (38.53-2.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.31 (at 2.90Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.226 , 0.249	Depositor
Wilson B-factor (Å <sup>2</sup> )	56.7	Xtriage
Anisotropy	0.313	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 53371 reflections	Xtriage
Total number of atoms	10919	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UNX, SEP

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	0/1844	0.55	0/2501
1	B	0.40	0/1846	0.55	0/2503
1	C	0.41	0/1837	0.56	0/2496
1	D	0.40	0/1803	0.54	0/2446
1	E	0.40	0/1841	0.55	0/2497
1	F	0.42	0/1363	0.56	0/1855
2	G	0.32	0/30	0.48	0/37
2	H	0.36	0/30	0.49	0/38
2	I	0.35	0/32	0.51	0/40
2	J	0.32	0/28	0.53	0/35
2	K	0.36	0/29	0.51	0/36
2	L	0.18	0/4	0.15	0/4
All	All	0.40	0/10687	0.55	0/14488

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1811	0	1694	8	0
1	B	1818	0	1710	7	0
1	C	1804	0	1675	7	0
1	D	1777	0	1642	7	0
1	E	1814	0	1710	9	0
1	F	1354	0	1052	4	0
2	G	42	0	35	0	0
2	H	42	0	33	1	0
2	I	44	0	40	0	0
2	J	40	0	28	0	0
2	K	41	0	30	0	0
2	L	15	0	7	0	0
3	M	100	0	22	0	0
3	N	45	0	11	0	0
3	O	50	0	12	0	0
3	V	65	0	15	0	0
4	A	10	0	0	0	0
4	B	18	0	0	0	0
4	C	14	0	0	0	0
4	D	9	0	0	0	0
4	E	5	0	0	0	0
4	F	1	0	0	0	0
All	All	10919	0	9716	31	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (31) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:13:LEU:HD11	1:D:82:VAL:HG22	1.84	0.58
1:D:28:LYS:HG3	1:D:103:LEU:HD21	1.87	0.56
1:A:13:LEU:HD11	1:C:82:VAL:HG22	1.89	0.54
1:A:28:LYS:HG3	1:A:103:LEU:HD21	1.91	0.52
1:D:96:VAL:O	1:D:100:VAL:HG23	2.10	0.52
1:B:63:ILE:HD11	1:D:17:ALA:HB2	1.92	0.52
1:B:28:LYS:HG3	1:B:103:LEU:HD21	1.92	0.52
1:E:28:LYS:HG3	1:E:103:LEU:HD21	1.93	0.51
1:C:28:LYS:HG3	1:C:103:LEU:HD21	1.91	0.51
1:E:63:ILE:HD11	1:F:17:ALA:HB2	1.93	0.51
1:B:82:VAL:HG22	1:D:13:LEU:HD11	1.92	0.50
1:E:96:VAL:O	1:E:100:VAL:HG23	2.12	0.49
1:B:17:ALA:HB2	1:D:63:ILE:HD11	1.95	0.48
1:E:17:ALA:HB2	1:F:63:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:63:ILE:HD11	1:C:17:ALA:HB2	1.96	0.47
1:A:96:VAL:O	1:A:100:VAL:HG23	2.14	0.47
1:A:82:VAL:HG22	1:C:13:LEU:HD11	1.98	0.46
1:E:132:ARG:HG3	1:E:186:ILE:HG13	2.01	0.43
1:E:60:TRP:CE2	1:E:137:VAL:HG12	2.55	0.42
1:A:132:ARG:HG3	1:A:186:ILE:HG13	2.02	0.41
1:B:179:TYR:HB3	1:B:196:LEU:HD21	2.02	0.41
1:C:132:ARG:HG3	1:C:186:ILE:HG13	2.02	0.41
1:D:60:TRP:CE2	1:D:137:VAL:HG12	2.55	0.41
1:E:13:LEU:HD11	1:F:82:VAL:HG22	2.02	0.41
1:E:179:TYR:HB3	1:E:196:LEU:HD21	2.03	0.41
1:E:78:LYS:O	1:E:82:VAL:HG23	2.21	0.41
1:A:60:TRP:CE2	1:A:137:VAL:HG12	2.57	0.40
1:B:233:TRP:HE1	2:H:226:ALA:HB2	1.86	0.40
1:F:96:VAL:O	1:F:100:VAL:HG23	2.22	0.40
1:C:60:TRP:CE2	1:C:137:VAL:HG12	2.56	0.40
1:A:81:MET:HE1	1:C:9:GLN:HG3	2.04	0.40

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	234/256 (91%)	232 (99%)	2 (1%)	0	100	100
1	B	232/256 (91%)	230 (99%)	2 (1%)	0	100	100
1	C	234/256 (91%)	231 (99%)	3 (1%)	0	100	100
1	D	233/256 (91%)	230 (99%)	3 (1%)	0	100	100
1	E	234/256 (91%)	231 (99%)	3 (1%)	0	100	100
1	F	194/256 (76%)	191 (98%)	3 (2%)	0	100	100
2	G	3/15 (20%)	3 (100%)	0	0	100	100
2	H	3/15 (20%)	3 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	3/15 (20%)	3 (100%)	0	0	100	100
2	J	3/15 (20%)	3 (100%)	0	0	100	100
2	K	3/15 (20%)	3 (100%)	0	0	100	100
All	All	1376/1611 (85%)	1360 (99%)	16 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	177/225 (79%)	174 (98%)	3 (2%)	73	94
1	B	181/225 (80%)	177 (98%)	4 (2%)	64	92
1	C	176/225 (78%)	171 (97%)	5 (3%)	56	90
1	D	167/225 (74%)	162 (97%)	5 (3%)	53	89
1	E	179/225 (80%)	178 (99%)	1 (1%)	92	98
1	F	86/225 (38%)	84 (98%)	2 (2%)	63	92
2	G	2/12 (17%)	2 (100%)	0	100	100
2	H	2/12 (17%)	2 (100%)	0	100	100
2	I	3/12 (25%)	3 (100%)	0	100	100
2	J	1/12 (8%)	1 (100%)	0	100	100
2	K	1/12 (8%)	1 (100%)	0	100	100
All	All	975/1410 (69%)	955 (98%)	20 (2%)	66	92

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLU
1	A	179	TYR
1	A	230	LEU
1	B	40	GLU
1	B	179	TYR

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Mol	Chain	Res	Type
1	B	207	GLU
1	B	230	LEU
1	C	29	ASN
1	C	40	GLU
1	C	179	TYR
1	C	212	ASN
1	C	230	LEU
1	D	29	ASN
1	D	40	GLU
1	D	87	GLU
1	D	179	TYR
1	D	230	LEU
1	E	179	TYR
1	F	35	GLU
1	F	80	GLU

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

Mol	Chain	Res	Type
1	B	6	GLN
1	C	106	ASN
1	D	106	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

6 non-standard protein/DNA/RNA residues are 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	SEP	G	228	2	9,9,10	6.07	2 (22%)	10,12,14	2.45	1 (10%)
2	SEP	H	228	2	9,9,10	6.35	2 (22%)	10,12,14	3.01	1 (10%)
2	SEP	I	228	2	9,9,10	6.06	2 (22%)	10,12,14	2.54	1 (10%)
2	SEP	J	228	2	9,9,10	6.18	1 (11%)	10,12,14	2.64	2 (20%)
2	SEP	K	228	2	9,9,10	6.25	2 (22%)	10,12,14	2.57	1 (10%)
2	SEP	L	228	2	9,9,10	6.16	2 (22%)	10,12,14	2.15	3 (30%)

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	SEP	G	228	2	-	0/6/8/10	0/0/0/0
2	SEP	H	228	2	-	0/6/8/10	0/0/0/0
2	SEP	I	228	2	-	0/6/8/10	0/0/0/0
2	SEP	J	228	2	-	0/6/8/10	0/0/0/0
2	SEP	K	228	2	-	0/6/8/10	0/0/0/0
2	SEP	L	228	2	-	0/6/8/10	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	228	SEP	O-C	18.81	1.24	1.11
2	K	228	SEP	O-C	18.54	1.24	1.11
2	J	228	SEP	O-C	18.29	1.24	1.11
2	L	228	SEP	O-C	18.14	1.23	1.11
2	I	228	SEP	O-C	17.97	1.23	1.11
2	G	228	SEP	O-C	17.96	1.23	1.11
2	L	228	SEP	CA-C	2.47	1.54	1.49
2	H	228	SEP	CA-C	2.08	1.53	1.49
2	K	228	SEP	CA-C	2.06	1.53	1.49
2	I	228	SEP	CA-C	2.05	1.53	1.49
2	G	228	SEP	CA-C	2.01	1.53	1.49

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	228	SEP	C-CA-N	-9.09	104.75	113.83
2	K	228	SEP	C-CA-N	-7.55	106.28	113.83
2	J	228	SEP	C-CA-N	-7.46	106.38	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	228	SEP	C-CA-N	-7.36	106.47	113.83
2	G	228	SEP	C-CA-N	-7.16	106.68	113.83
2	L	228	SEP	OG-CB-CA	4.80	115.14	108.64
2	L	228	SEP	P-OG-CB	-2.97	111.03	118.63
2	L	228	SEP	C-CA-N	-2.44	111.39	113.83
2	J	228	SEP	O3P-P-O2P	2.03	115.01	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 57 ligands modelled in this entry, 57 are unknown - 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.

## 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.