



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 31, 2020 – 10:03 AM BST

PDB ID : 1F51
Title : A TRANSIENT INTERACTION BETWEEN TWO PHOSPHORELAY PROTEINS TRAPPED IN A CRYSTAL LATTICE REVEALS THE MECHANISM OF MOLECULAR RECOGNITION AND PHOSPHOTRANSFER IN SINGAL TRANSDUCTION
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Deposited on : 2000-06-11
Resolution : 3.00 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
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)	:	2.13

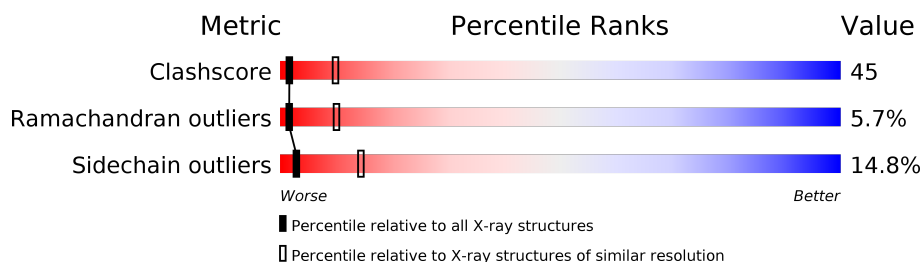
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	182	
1	B	182	
1	C	182	
1	D	182	
2	E	119	
2	F	119	
2	G	119	
2	H	119	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9751 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 SPORULATION INITIATION PHOSPHOTRANSFERASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	0	0
			1489	949	250	283	7			
1	B	182	Total	C	N	O	S	6	0	0
			1504	959	253	285	7			
1	C	181	Total	C	N	O	S	0	0	0
			1481	945	249	280	7			
1	D	182	Total	C	N	O	S	6	0	0
			1497	955	252	283	7			

- Molecule 2 is a protein called SPORULATION INITIATION PHOSPHOTRANSFERASE F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	119	Total	C	N	O	S	0	0	0
			940	603	155	177	5			
2	F	119	Total	C	N	O	S	0	0	0
			950	609	156	180	5			
2	G	119	Total	C	N	O	S	0	0	0
			947	608	155	179	5			
2	H	119	Total	C	N	O	S	0	0	0
			940	603	155	177	5			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

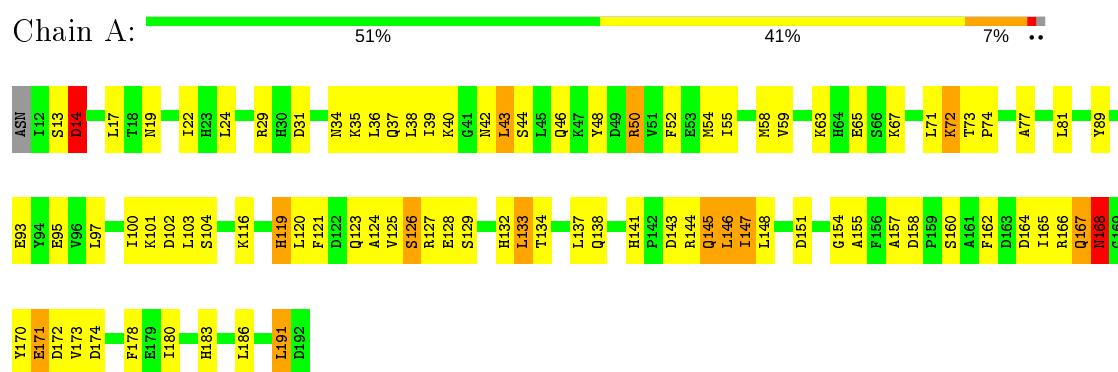
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

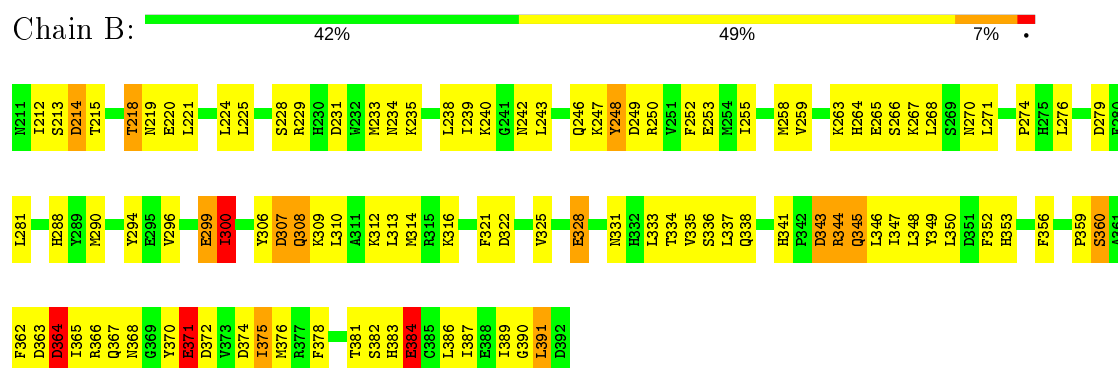
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

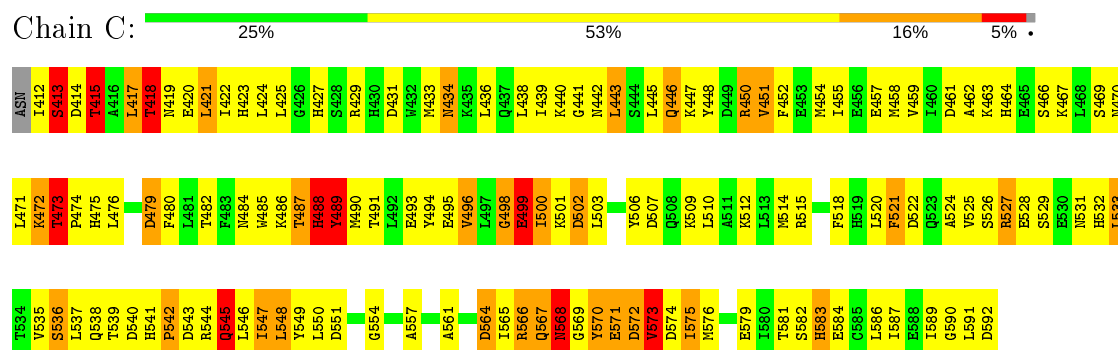
• Molecule 1: SPORULATION INITIATION PHOSPHOTRANSFERASE B



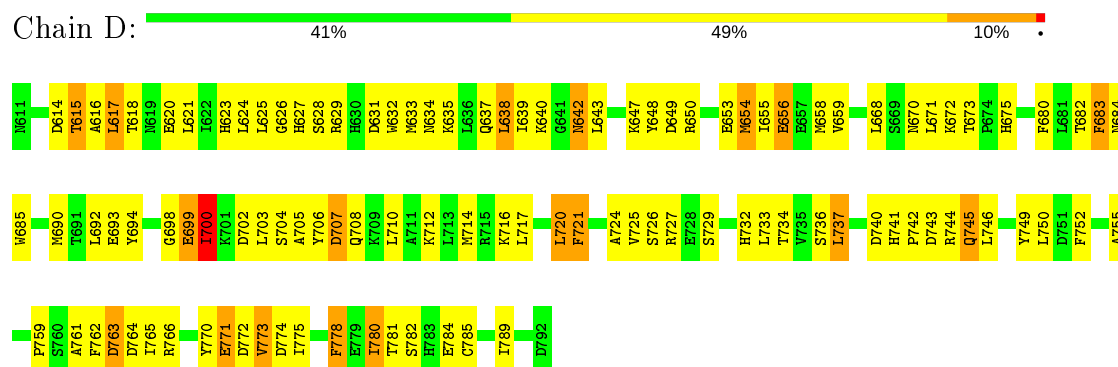
• Molecule 1: SPORULATION INITIATION PHOSPHOTRANSFERASE B



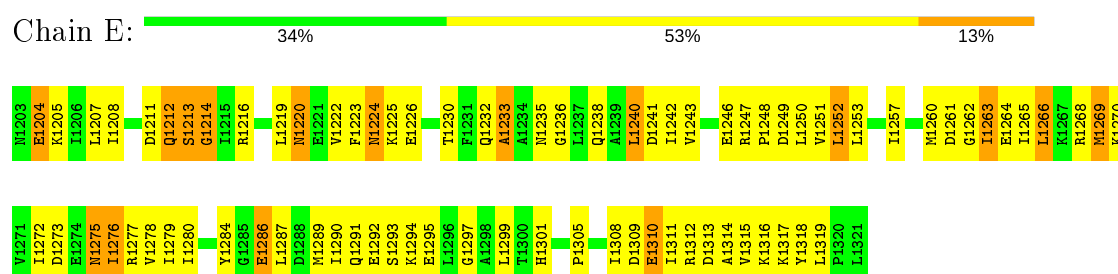
• Molecule 1: SPORULATION INITIATION PHOSPHOTRANSFERASE B



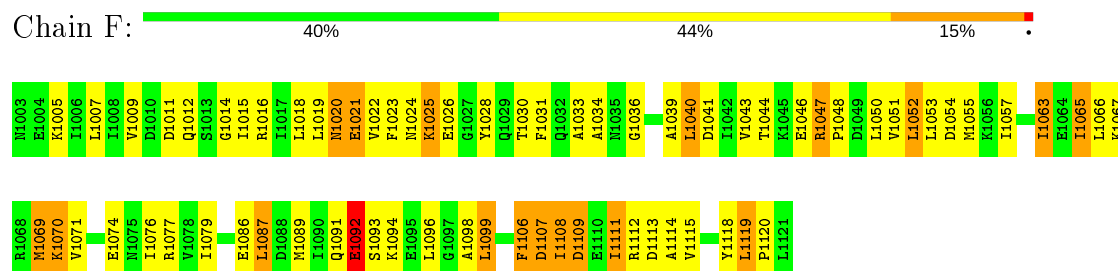
• Molecule 1: SPORULATION INITIATION PHOSPHOTRANSFERASE B



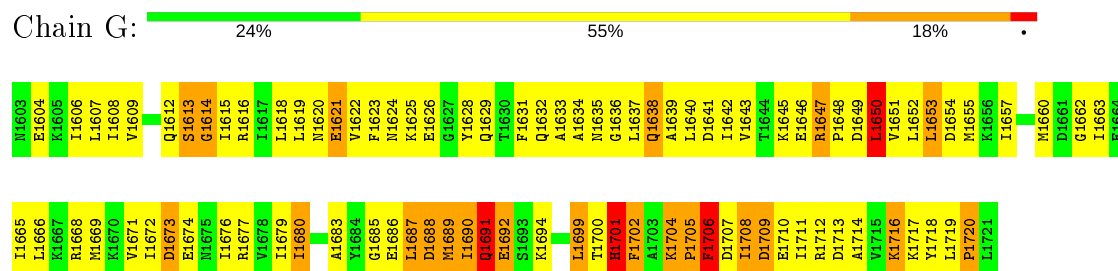
• Molecule 2: SPORULATION INITIATION PHOSPHOTRANSFERASE F



• Molecule 2: SPORULATION INITIATION PHOSPHOTRANSFERASE F



• Molecule 2: SPORULATION INITIATION PHOSPHOTRANSFERASE F



• Molecule 2: SPORULATION INITIATION PHOSPHOTRANSFERASE F



K1467	K1403
R1468	E1404
M1469	K1405
K1470	I1406
V1471	L1407
I1472	I1408
D1473	V1409
	D1410
	D1411
I1476	Q1412
R1477	S1413
V1478	G1414
I1479	I1415
I1480	R1416
M1481	I1417
T1482	L1418
A1483	L1419
	N1420
E1486	E1421
L1487	V1422
	F1423
I1490	N1424
	K1425
K1494	E1426
E1495	G1427
L1496	I1428
G1497	
A1498	F1431
L1499	Q1432
T1500	A1433
H1501	
	G1436
P1505	L1437
F1506	Q1438
D1507	A1439
I1508	L1440
D1509	D1441
E1510	I1442
I1511	V1443
R1512	T1444
D1513	K1445
A1514	E1446
V1515	R1447
K1516	P1448
K1517	D1449
Y1518	L1450
L1519	V1451
P1520	L1452
L1521	L1453
	D1454
	M1455
	G1459
	D1460
	D1461
	G1462
	I1463
	E1464
	I1465
	L1466

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.97Å 117.77Å 170.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 3.00	Depositor
% Data completeness (in resolution range)	88.7 (45.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	7.60	Depositor
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.228 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9751	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.45	0/1522	0.74	2/2056 (0.1%)
1	B	0.50	1/1537 (0.1%)	0.78	1/2075 (0.0%)
1	C	0.46	0/1514	0.96	8/2045 (0.4%)
1	D	0.45	0/1530	0.74	1/2065 (0.0%)
2	E	0.42	0/951	0.77	0/1280
2	F	0.48	0/961	0.81	2/1293 (0.2%)
2	G	0.48	0/958	0.90	3/1289 (0.2%)
2	H	0.42	0/951	0.98	7/1280 (0.5%)
All	All	0.46	1/9924 (0.0%)	0.83	24/13383 (0.2%)

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	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	384	GLU	CD-OE2	7.28	1.33	1.25

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	567	GLN	N-CA-C	-10.70	82.12	111.00
2	G	1705	PRO	N-CA-C	-10.66	84.38	112.10
1	C	488	HIS	N-CA-C	7.60	131.52	111.00
2	H	1520	PRO	N-CA-C	6.97	130.22	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1519	LEU	N-CA-C	-6.78	92.70	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	570	TYR	Sidechain

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	1489	0	1437	83	0
1	B	1504	0	1463	113	0
1	C	1481	0	1419	169	0
1	D	1497	0	1449	121	1
2	E	940	0	970	85	1
2	F	950	0	987	80	0
2	G	947	0	983	156	0
2	H	940	0	970	112	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
All	All	9751	0	9678	867	1

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 45.

The worst 5 of 867 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:H:1465:ILE:O	2:H:1469:MET:HB2	1.40	1.19
1:C:520:LEU:HD13	1:C:565:ILE:HD11	1.27	1.15
1:C:544:ARG:HH21	1:C:592:ASP:HA	1.10	1.14
2:G:1677:ARG:HB3	2:G:1699:LEU:HD11	1.31	1.13
2:G:1683:ALA:HA	2:G:1704:LYS:HE3	1.28	1.13

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
1:D:743:ASP:O	2:E:1294:LYS:NZ[4_565]	1.99	0.21

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	179/182 (98%)	154 (86%)	22 (12%)	3 (2%)	9	39
1	B	180/182 (99%)	148 (82%)	24 (13%)	8 (4%)	2	15
1	C	179/182 (98%)	139 (78%)	23 (13%)	17 (10%)	0	3
1	D	180/182 (99%)	145 (81%)	27 (15%)	8 (4%)	2	15
2	E	117/119 (98%)	94 (80%)	19 (16%)	4 (3%)	3	20
2	F	117/119 (98%)	101 (86%)	13 (11%)	3 (3%)	5	27
2	G	117/119 (98%)	79 (68%)	26 (22%)	12 (10%)	0	2
2	H	117/119 (98%)	89 (76%)	15 (13%)	13 (11%)	0	2
All	All	1186/1204 (98%)	949 (80%)	169 (14%)	68 (6%)	1	10

5 of 68 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	168	ASN
1	B	248	TYR
1	B	300	ILE
1	B	307	ASP

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	164/167 (98%)	149 (91%)	15 (9%)	9	34
1	B	167/167 (100%)	148 (89%)	19 (11%)	5	24
1	C	161/167 (96%)	122 (76%)	39 (24%)	0	3
1	D	165/167 (99%)	149 (90%)	16 (10%)	8	31
2	E	102/105 (97%)	88 (86%)	14 (14%)	3	17
2	F	105/105 (100%)	82 (78%)	23 (22%)	1	5
2	G	104/105 (99%)	86 (83%)	18 (17%)	2	10
2	H	102/105 (97%)	88 (86%)	14 (14%)	3	17
All	All	1070/1088 (98%)	912 (85%)	158 (15%)	3	14

5 of 158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	581	THR
1	D	780	ILE
2	H	1440	LEU
1	D	617	LEU
1	D	720	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	708	GLN
2	E	1224	ASN
2	H	1438	GLN
1	D	732	HIS
2	E	1238	GLN

5.3.3 RNA ⓘ

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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 [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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.