



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:20 PM GMT

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
<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) : **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

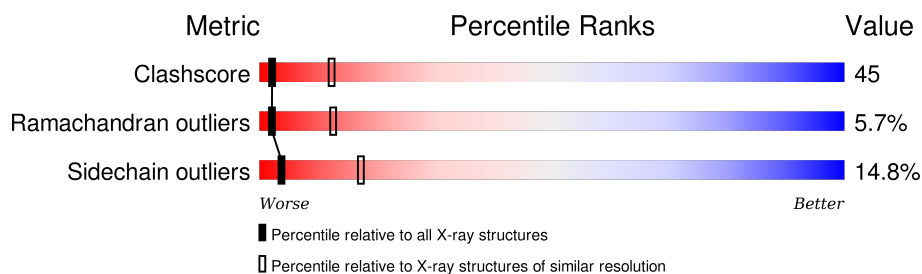
1 Overall quality at a glance

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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

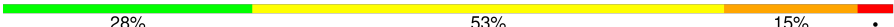
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey 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 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	

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Mol	Chain	Length	Quality of chain
2	H	119	 A horizontal bar chart showing the quality of chain H. The bar is divided into four segments: green (28%), yellow (53%), orange (15%), and red (4%). The segments are labeled with their respective percentages: 28%, 53%, 15%, and a small red segment at the end. A small black dot is visible at the end of the red segment.

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).

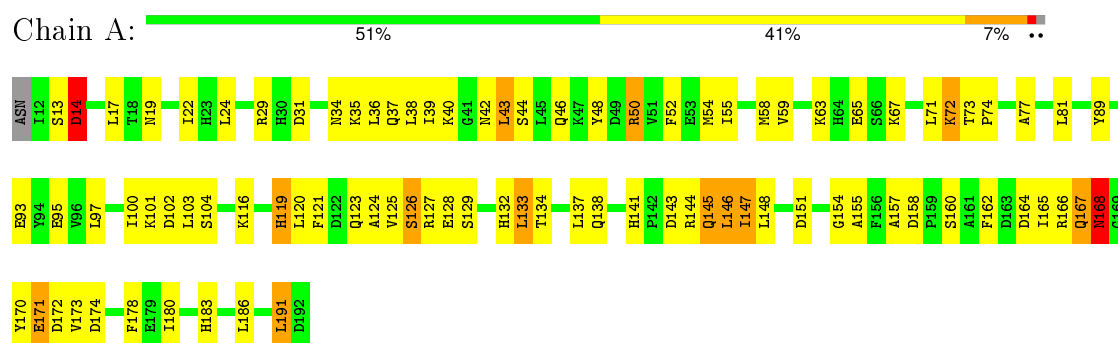
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

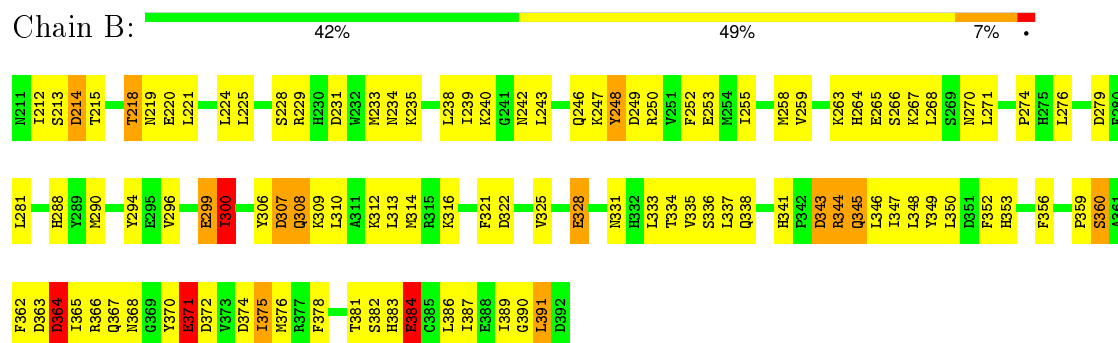
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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.

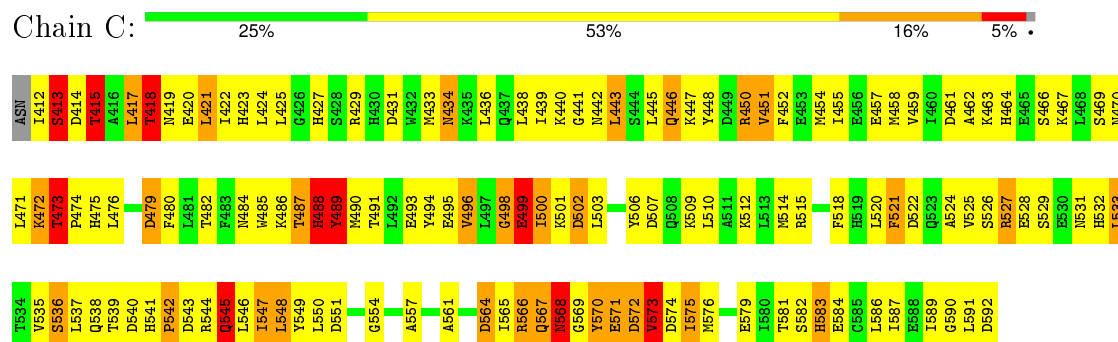
• Molecule 1: SPORULATION INITIATION PHOSPHOTRANSFERASE B



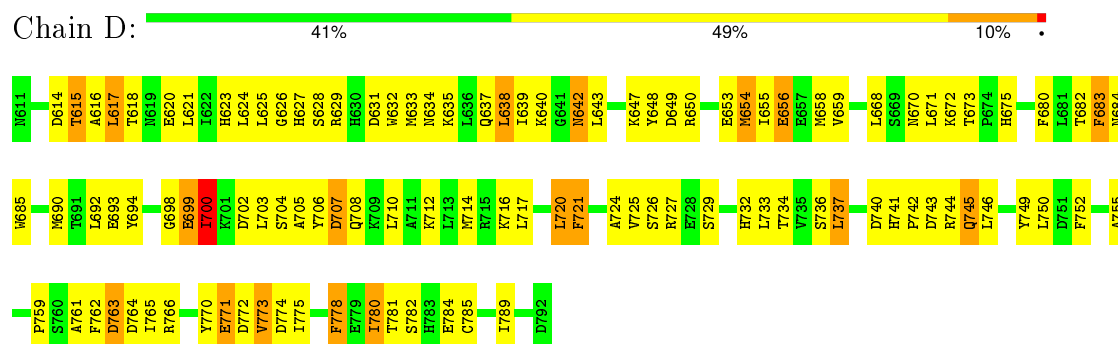
• Molecule 1: SPORULATION INITIATION PHOSPHOTRANSFERASE B



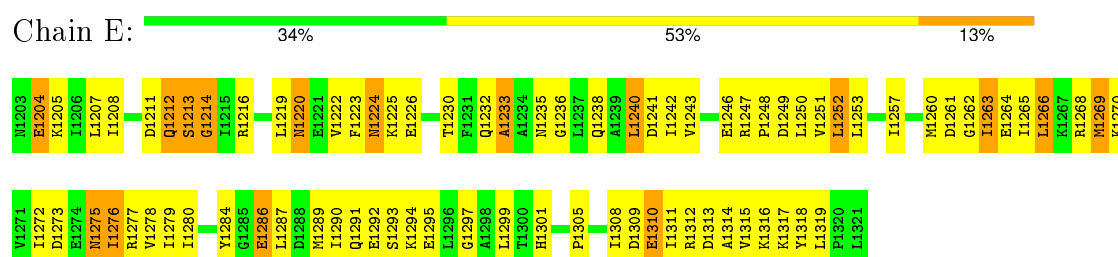
• Molecule 1: SPORULATION INITIATION PHOSPHOTRANSFERASE B



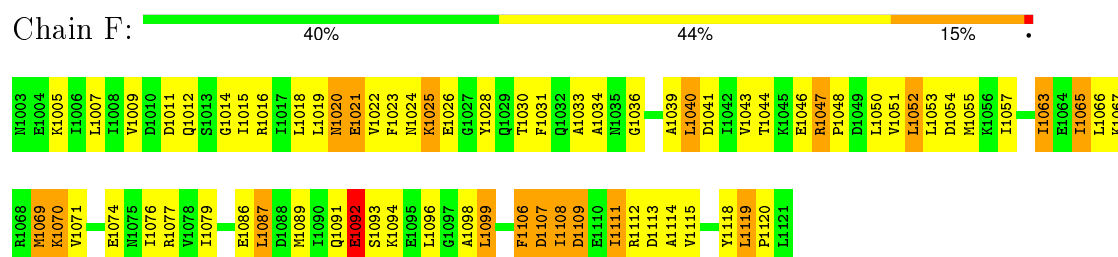
● Molecule 1: SPORULATION INITIATION PHOSPHOTRANSFERASE B



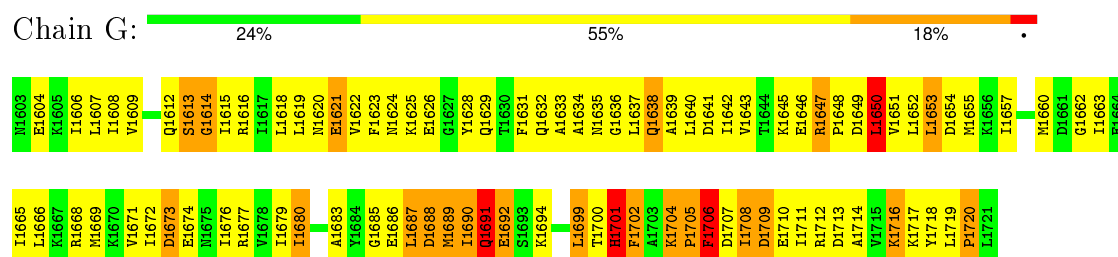
● Molecule 2: SPORULATION INITIATION PHOSPHOTRANSFERASE F



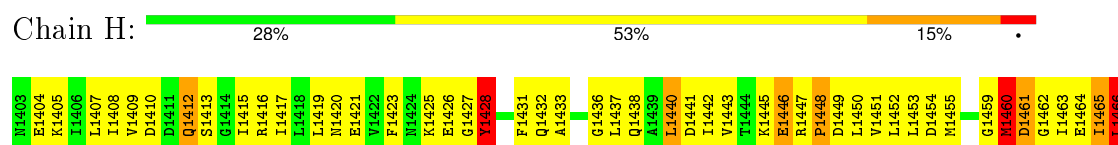
● Molecule 2: SPORULATION INITIATION PHOSPHOTRANSFERASE F



● Molecule 2: SPORULATION INITIATION PHOSPHOTRANSFERASE F



● Molecule 2: SPORULATION INITIATION PHOSPHOTRANSFERASE F



K1467	R1468	M1469	K1470	V1471	I1472	D1473	I1476	R1477	V1478	I1479	I1480	M1481	T1482	A1483	E1486	L1487	I1490	K1494	E1495	I1496	G1497	A1498	L1499	T1500	H1501	P1505	F1506	D1507	I1508	D1509	E1510	I1511	R1512	D1513	A1514	V1515	K1516	K1517	Y1518	L1519	P1520	L1521
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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 [i](#)

5.1 Standard geometry [i](#)

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%)	11	46
1	B	180/182 (99%)	148 (82%)	24 (13%)	8 (4%)	3	18
1	C	179/182 (98%)	139 (78%)	23 (13%)	17 (10%)	1	3
1	D	180/182 (99%)	145 (81%)	27 (15%)	8 (4%)	3	18
2	E	117/119 (98%)	94 (80%)	19 (16%)	4 (3%)	5	25
2	F	117/119 (98%)	101 (86%)	13 (11%)	3 (3%)	7	33
2	G	117/119 (98%)	79 (68%)	26 (22%)	12 (10%)	1	3
2	H	117/119 (98%)	89 (76%)	15 (13%)	13 (11%)	0	2
All	All	1186/1204 (98%)	949 (80%)	169 (14%)	68 (6%)	2	12

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%)	12	41
1	B	167/167 (100%)	148 (89%)	19 (11%)	7	28
1	C	161/167 (96%)	122 (76%)	39 (24%)	1	4
1	D	165/167 (99%)	149 (90%)	16 (10%)	10	37
2	E	102/105 (97%)	88 (86%)	14 (14%)	4	20
2	F	105/105 (100%)	82 (78%)	23 (22%)	1	6
2	G	104/105 (99%)	86 (83%)	18 (17%)	2	12
2	H	102/105 (97%)	88 (86%)	14 (14%)	4	20
All	All	1070/1088 (98%)	912 (85%)	158 (15%)	4	17

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 carbohydrates 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 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.