WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Aug 2, 2023 – 09:11 PM EDT

PDB ID : 1F51
Title : A TRANSIENT INTERACTION BETWEEN TWO PHOSPHORELAY
PROTEINS TRAPPED IN A CRYSTAL LATTICE REVEALS THE MECH-
ANISM OF MOLECULAR RECOGNITION AND PHOSPHOTRANSFER
IN SINGAL TRANSDUCTION
Authors : Zapf, J.; Sen, U.; Madhusudan, M.; Hoch, J.A.; Varughese, K.I.
Deposited on : 2000-06-11
Resolution : 3.00 Å(reported)

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

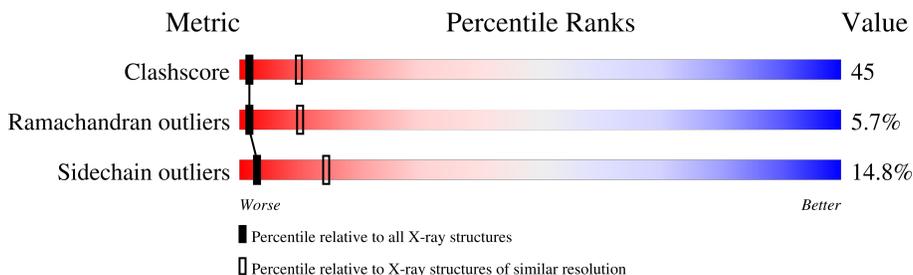|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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	Percentile Ranks	Value
Clashscore		45
Ramachandran outliers		5.7%
Sidechain outliers		14.8%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

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 of 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	182	51% 41% 7% ••
1	B	182	42% 49% 7% •
1	C	182	25% 53% 16% 5% •
1	D	182	41% 49% 10% •
2	E	119	34% 53% 13%
2	F	119	40% 44% 15% •
2	G	119	24% 55% 18% •
2	H	119	28% 53% 15% •

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 1489	C 949	N 250	O 283	S 7	0	0	0
1	B	182	Total 1504	C 959	N 253	O 285	S 7	6	0	0
1	C	181	Total 1481	C 945	N 249	O 280	S 7	0	0	0
1	D	182	Total 1497	C 955	N 252	O 283	S 7	6	0	0

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

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

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

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

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.
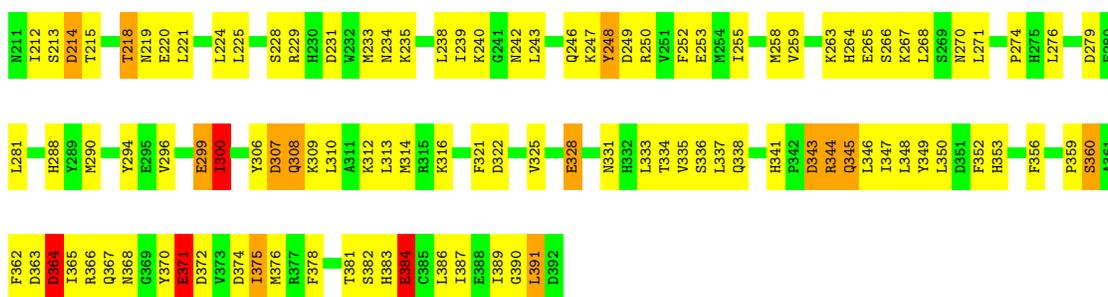
Note EDS was not executed.

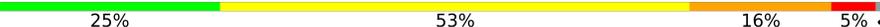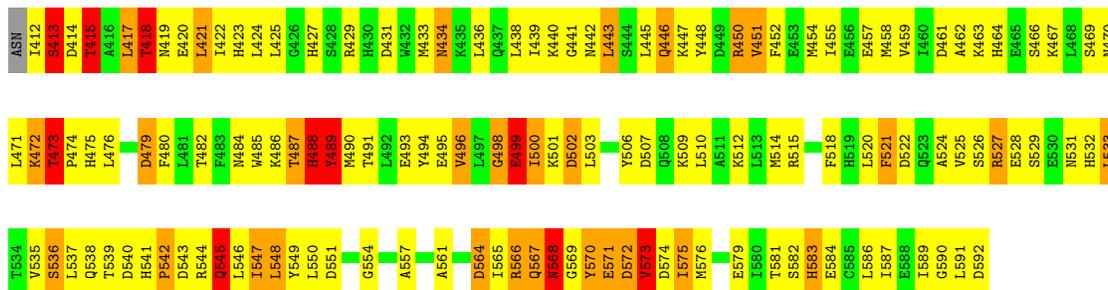• Molecule 1: SPORULATION INITIATION PHOSPHOTRANSFERASE B

Chain A:
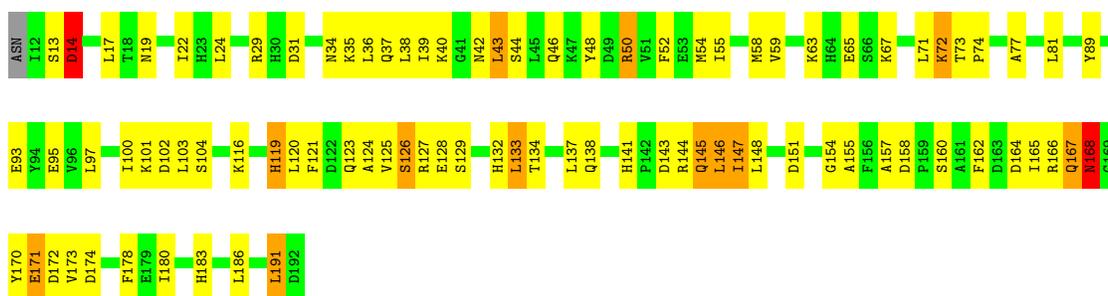
• Molecule 1: SPORULATION INITIATION PHOSPHOTRANSFERASE B

Chain B:

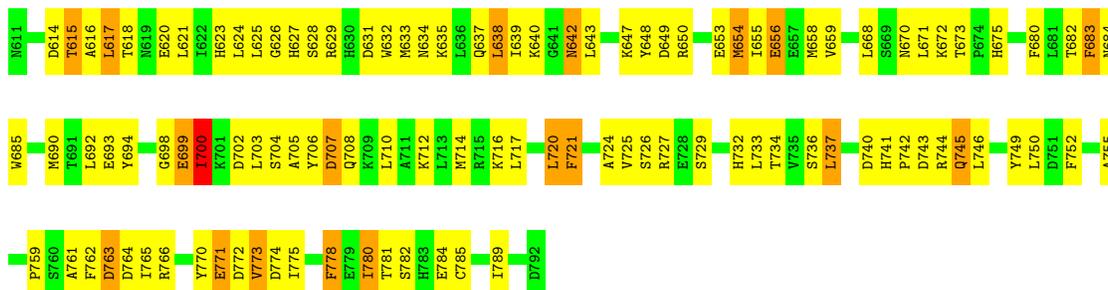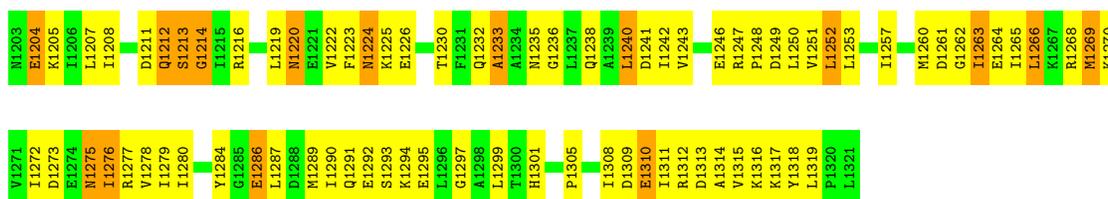• Molecule 1: SPORULATION INITIATION PHOSPHOTRANSFERASE B

Chain C:

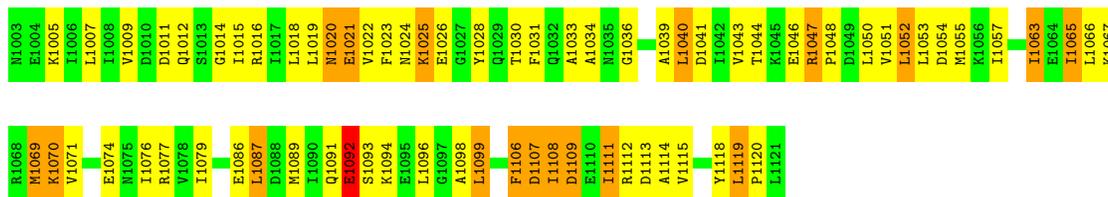• Molecule 1: SPORULATION INITIATION PHOSPHOTRANSFERASE B

Chain D:

• Molecule 2: SPORULATION INITIATION PHOSPHOTRANSFERASE F

Chain E:

• Molecule 2: SPORULATION INITIATION PHOSPHOTRANSFERASE F

Chain F:

• Molecule 2: SPORULATION INITIATION PHOSPHOTRANSFERASE F

Chain G:

• Molecule 2: SPORULATION INITIATION PHOSPHOTRANSFERASE F

Chain H:

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 (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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 ⓘ

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 ⓘ

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	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
2	F	1074	GLU
2	G	1709	ASP
2	F	1106	PHE
2	G	1650	LEU
2	H	1466	LEU

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

Mol	Chain	Res	Type
2	E	1291	GLN
2	G	1632	GLN
2	F	1020	ASN
2	G	1612	GLN
2	G	1691	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

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 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.